Analysis of the Limit Resolution of Grating Spectrometer

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Abstract. As a matter of fact, grating spectrometer has been widely used in various applications in recent years on account of its simple structure and high accuracy. On this basis, this study introduces the research history and development status of grating spectrometer in the last hundred years. To optimize the resolution of the grating spectrometer, the design of the instrument, the selection of optical elements, the stability of the light source and the performance of the detector should be considered comprehensively. The limit resolution in the visible range is affected by the number of lines of the grating and the quality of the optical element. In the UV range its resolution depends on the grating parameters and instrument design. The limiting resolution in the infrared range is limited by the wavelength range and the quality of the optical element. In addition, this research also involves the realization and progress of some related advanced technologies. Some hypotheses for improving the resolution of the grating spectrometer are also presented and proposed.

Keywords: Limit resolution, grating spectrometer, visible band, infrared band, ultraviolet band.

1. Introduction

Although grating spectrometers were widely used in industry only in the last century, human efforts to study spectroscopy and improve the resolution of grating began in the 19th century [1-3]. In 1802, British physicist William Hyde Wollaston discovered discontinuities in the solar spectrum, which appeared as many dark lines in the spectrum. These dark lines, now called Fraunhofer lines, were rediscovered and accurately described by the German physicist Joseph von Fraunhofer. von Fraunhofer built the first diffraction grating consisting of 260 tightly parallel wires in 1821, and later modified the grating with glass made of gold-plated corundum to achieve a finer groove spacing of up to 300 gr/mm. In New York, Lewis Rutherfurd produced a reflective grating using polished mirror metal in the 1870s that could reach 680 gr/mm. At the same time, Lord Rayleigh proposed the photographic reproduction of gratings in order to enable mass production. Henry Rowland of Johns Hopkins University has modified the screws used in the grating to eliminate some of the errors in the spectrometer. Robert Wood, also of Johns Hopkins University, invented the blazed grating in 1910. The aluminized glass reflectors developed by John Strong in the early 1930s using vacuum deposition technology provided new possibilities and directions for later grating production. In the 1960s, holographic gratings were developed based on the monochromatic laser interference phenomenon. The volume phase holographic gratings developed in recent years can periodically adjust the refractive index in thin gelatin layers.

Since the development of grating spectrometer, the application field has been very wide, involving physics, astronomy, chemistry, biology, medicine, and other scientific fields, as well as optical fiber communication, industrial production and other fields. In the field of physics, grating spectrometer can study the fine structure in visible light of plasma. In the field of astronomy, it can detect and quantify the gas content and isotopes of planets or atmospheres. In the field of biology, it can analyze the structure and function of biological molecules. High-resolution spectrometers to accurately measure the optical signal-to-noise ratio of density wavelength-division multiplexing (DWDM) systems [4]. Nowadays, according to Zhou’s introduction, there are two directions for the development of grating spectrometers: the first is to continue to improve the resolution of grating spectrometers, and the second is to miniaturize the instrument [5].

This paper hopes to have a more comprehensive grasp and presentation of the research history and status of grating spectrometer, and promote researchers to further improve the grating spectrometer.

2. Structure of Spectrometer

Grating spectrometer is a kind of optical instrument which uses a plane grating or a flat field concave grating and uses the diffraction principle of light to divide the light. Grating spectrometer is often used in color measurement, chemical composition concentration measurement, gas composition analysis and other fields. At present, the flat-field concave grating spectrometer is more common. The structure of grating spectrometer consists of light source, sample chamber, grating spectrometer and detection system. The most important system is the grating monochromator. It plays the role of dispersing the measured polychromatic light. It is mainly composed of an entrance slit, a grating, two collimating mirrors and an exit slit.

The blazed grating is a reflective grating with a zigzag surface with smooth grooves. There are two coefficients that need to be noticed, and these two coefficients are only relevant to themselves. The first coefficient is called the flare angle, which is the angle between the groove surface and the plane. The second coefficient is called the flare wavelength, and it is the wavelength corresponding to the maximum intensity of light. It is related to grating constant (groove spacing) and flare Angle. Seen from Fig. 1, the incidence Angle is α, the diffraction Angle is θ, the flare Angle is β, and the grating coefficient is d [6].

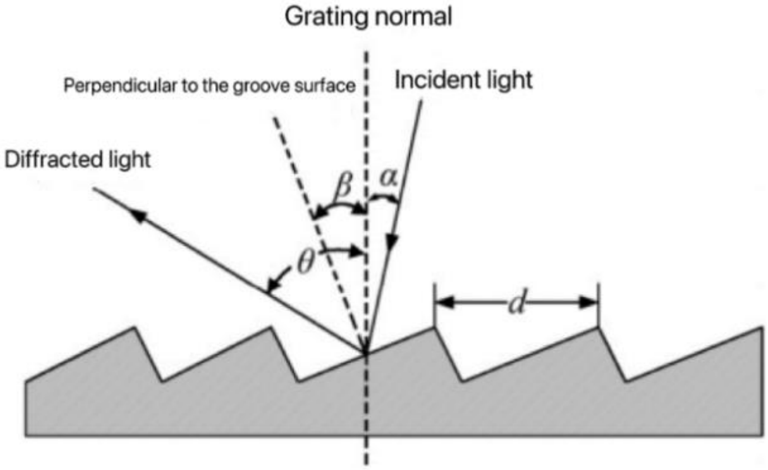

Figure 1. Diffraction schematic of a blazed grating [6].

According to the grating equation, we can get:

$$d(\sin\alpha + \sin\theta) = n\lambda \tag{1}$$

When $\alpha = \theta = \beta$, the diffraction intensity is the largest, that is, $2d\sin\beta = n\lambda_b$, λ_b is the shining wavelength. The working flow of the grating spectrometer is that the light emitted from the light source passes through the sample chamber, enters the incident slit, is reflected in the first collimating mirror, and then the light is diffracted in the blazed grating for splitting, and then reflected in the second collimating mirror, and finally enters the exit slit, and enters the detection system for spectral analysis. The resolution of grating spectrometer is affected by many factors, such as the width of incident slit and the number of total grating slit [6, 7]. The formula of grating resolution is always:

$$R = \frac{\lambda}{d\lambda} \tag{2}$$

The linear dispersion rate of the grating is:

$$D_l = \frac{fd\theta}{d\lambda} = \frac{jf}{d\,cos\,\theta} \tag{3}$$

Here, f is the focal length. The angular distance between the two lines is

$$\Delta\theta = \frac{\lambda}{Nd\cos\theta} \tag{4}$$

Where, N is the total number of grating gaps. According to Rayleigh criterion, when two spectral lines of the same intensity, the center of one spectral line just appears on the dark line of the other spectral line, it can just be distinguished. The minimum resolution wavelength is

$$d\lambda = \frac{\Delta\theta}{D_l} = \frac{\lambda}{jN} \tag{5}$$

Therefore, the grating resolution is:

$$R = jN \tag{6}$$

The resolution of the grating spectrometer is proportional to the number of cracks and spectral order of the grating. In practice, the width of the entrance slit must also be considered as $R \propto 1/L$ where L is the width of the entrance slit. Therefore, the grating resolution is affected by the size of the incident slit and the total number of grating gaps. As the incidence slit decreases, the resolution increases. As the grating has more and more gaps, the grating resolution will increase. It should be noted that, taking into account the size of the actual instrument, as well as being restricted by diffraction phenomena, the resolution will inevitably appear the maximum limit.

3. Resolution and Application

In this part, the application scenarios of grating spectrometer in visible, ultraviolet and infrared bands are introduced in detail.

3.1. Visible Band

The visible wavelength range is about 400 to 760nm, and it also has many applications, such as Raman spectroscopy and plasma radiation. Raman spectroscopy is developed based on the Raman scattering effect of incident light and scattered light at different frequencies. By analyzing the scattering spectra of the molecules studied by excitation light radiation, it can analyze the information of molecular structure, such as the vibration and rotation of molecules. The wavelength of the Raman spectrum ranges from 200 to 800nm. According to Wu’s instruction, the advantage of this technology is that the scattering spectrum of the substance is only related to the structure of the substance, with high sensitivity and the detection of multiple components of the substance (seen from Fig. 2) [8]. At the same time, Wu also mentioned that there are two main methods to improve the resolution of the current Raman spectrometer, which physical methods include coded aperture method and analog optical slice method and the numerical method relies on the deconvolution calculation of the scattering spectra obtained. Because Raman scattering is much smaller than Rayleigh scattering, the weak signal needs to be denoised to improve the signal-to-noise ratio. According to other scholars, they used high-resolution spectrometers in their research to conduct detailed studies of the fine structure of the visible band in the plasma emission spectrum [9].

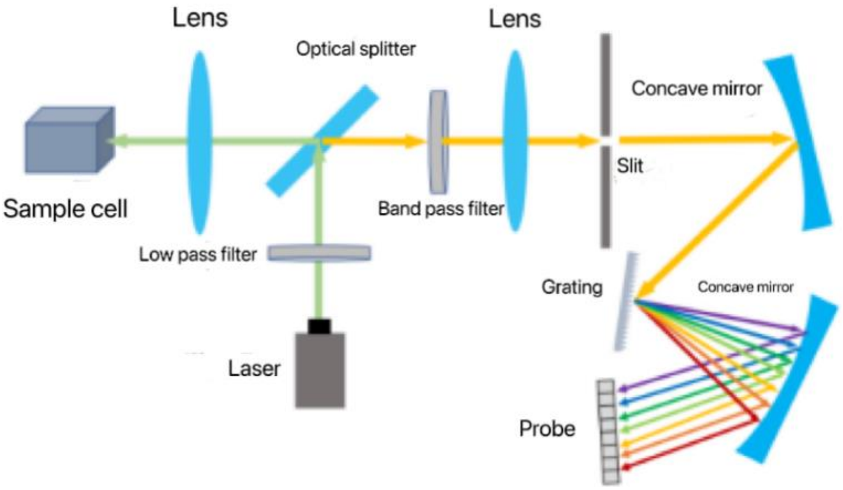

Figure 2. Structure of grating dispersive Raman spectrometer [8].

3.2. UV Band

Usually, the wavelength range of what we call the ultraviolet spectrum is mainly 200 ~ 800nm. In the ultraviolet absorption spectrum, electron transitions are $\sigma \rightarrow \sigma^*$, $n \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$. In UV absorption spectrometry, there is a quantitative relationship between absorbance and substance concentration at selected wavelengths. This relationship is often described as the Beer-Lambert Law.

$$A = \varepsilon c L = -log(I/I0) \tag{7}$$

It states that at a particular wavelength, the absorbance is proportional to the product of the substance's concentration and the light path. Molar absorption coefficient is an inherent property of a specific substance at a specific wavelength, reflecting its ability to absorb light. The linear relationship of the Beer-Lambert law usually holds over a lower concentration range.

Hoadley et al. pointed out that sensitive observations in ultraviolet conditions are difficult because UV optical performance and imaging efficiency lag behind their visible and infrared counterparts [10]. Because UV optical performance and imaging efficiency are not as good as the corresponding characteristics of visible light and infrared light, it is difficult to make accurate observations in ultraviolet conditions. According to Sun et al., near-space data on the UV-radiation background of the upper atmosphere is a major scientific goal for our country [11]. The factors that affect the ultraviolet absorption spectrum of organic compounds are internal (conjugation, steric hindrance, chromic effect, etc.) and external (solvent effects such as solvent polarity, acid, and alkali). The ultraviolet light band can measure the vibrational electron spectrum that absorbs a variety of trace gases more accurately. It can significantly reduce cross interference due to scattering processes, or other absorption, to improve sensitivity (as shown in Table 1). In addition, because the dust in the atmosphere will scatter and absorb ultraviolet light, the luminous flux and mobility are greatly reduced, which will affect the resolution of the instrument. Today's grating spectrometers, which typically use high-resolution FPI spectrometers, have a lower signal-to-noise ratio. It is generally used for atmospheric trace gases and their isotopic isomers, for qualitative and quantitative analysis of polymers and small molecules, and for molecular analysis with conjugated systems. It is also frequently used in observations and experiments on astrophysical systems. The UV-VIS absorption spectrum can be used to determine the unsaturated groups in organic compounds, and to distinguish the configuration, conformation and isomers of the compounds [11].

Table 1. Uncertainties of the MN-UVS absolute radiometric calibration.

Parameters	Uncertainties				
	λ = 200 nm	λ = 250 nm	λ = 300 nm	λ = 350 nm	λ = 400 nm
Temporal stability of the UV source	0.1%	0.1%	0.1%	0.1%	0.1%
Irradiance uncertainty of the UV light source	5.50%	2.04%	1.87%	1.86%	1.77%
Non-uniform of the UV source	1.15%	1.15%	1.15%	1.15%	1.15%
Reflectivity uncertainty of the diffuser	0.50%	0.50%	0.50%	0.50%	0.50%
Uncertainty of the distance	0.58%	0.58%	0.58%	0.58%	0.58%
Non-uniform of the MN-UVS	0.50%	0.50%	0.50%	0.50%	0.50%
Nonlinearity of the detector	0.58%	0.58%	0.58%	0.58%	0.58%
Uncertainty of the gain of the ICCD	1.5%	1.5%	1.5%	1.5%	1.5%
Noise	1.15%	1.15%	1.15%	1.15%	1.15%
Uncertainty of the spectral calibration	0.15%	0.12%	0.10%	0.08%	0.07%
Overall extended uncertainty (*k*=2)	12.0%	6.4%	6.2%	6.1%	6.0%
Overall standard uncertainty (*k*=1)	6.0%	3.2%	3.1%	3.1%	3.0%

3.3. Infrared Band

Infrared light can be divided into near infrared, middle infrared and far infrared light. Infrared spectrometers are generally divided into two categories, one is raster scanning, rarely used; The other is a Michelson interferometer scan, called Fourier transform infrared spectroscopy, which is currently more widely used. If the vibration frequency of a certain group in the molecule is consistent with the irradiated infrared frequency, it will generate resonance and absorb a certain amount of infrared light, and then the spectrum is obtained after processing. The absorption of infrared spectrum is mainly related to the vibration and rotation of molecules.

According to Yang's study, in the infrared light band, its limiting resolution is affected by the maximum optical path difference, stability and reduced luminous flux [12]. The use of high brightness and good stability of the infrared light source can improve the resolution. The application of advanced light source technologies such as lasers also helps to improve the performance of spectrometers. The sensitivity and response speed of the detector of the infrared spectrometer are also key factors. Using thinner samples and finer sampling techniques can improve resolution. Advanced infrared detector technology, such as photodiode arrays (PDAs), semiconductor detectors, etc., can improve the signal-to-noise ratio and response speed, thereby contributing to improved resolution. The stability of the instrument is very important for long-term spectral acquisition and measurement. Instruments with poor stability may lead to peak shape change and wave number drift, affecting resolution. Reasonable design of optical path can reduce the difference of optical path and improve the resolution. In the study of Pang et al., the method of using double grating is mentioned, so that the light can be reflected four times and improve the luminous flux (seen from Fig. 3) [13]. Infrared spectral absorption is widely used in chemical analysis. It can be used to identify and verify the structure of a compound, determine the types of functional groups and chemical bonds in the molecule. It is capable of detecting material defects, impurities and crystal structures, as well as surface and interface properties. Infrared spectral absorption is used to verify the quality and purity of the drug. It can be used to analyze the structure of drug molecules.

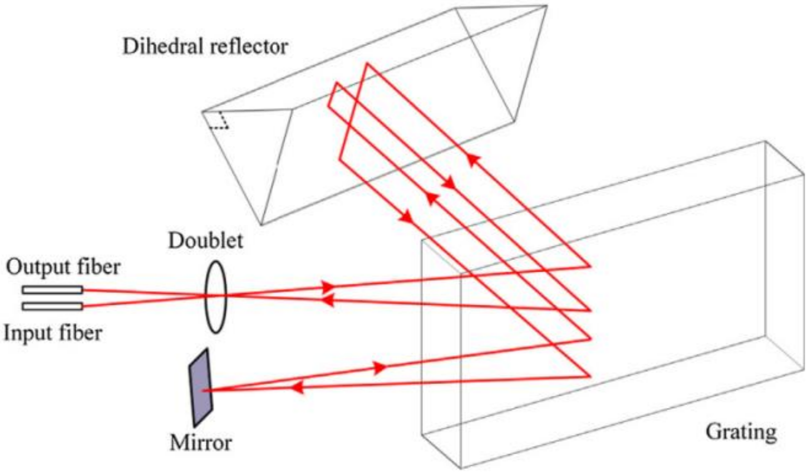

Figure 3. Principle of the grating multiplexing structure-based spectrometer [13].

4. Limitations & Prospects

At present, the resolution of grating spectrometers is limited by several major factors. We already know that the higher the spectral resolution, the narrower the spectral band detected. Hence, there is a certain contradiction between high resolution and wide spectrum. In the design of the spectrometer, people need to reasonably balance the three important indicators of spectral resolution, spectral range, and spectrometer volume, only focusing on a single indicator for optimization, will inevitably lead to the lack of other indicators. One should fully consider the effects of spherical aberration, coma, and astigmatism on the imaging quality of the spectrometer system. Firstly, the resolution of a grating spectrometer is related to its grating constant. The grating constant determines the spacing of the lines in the grating, which affects the resolution of the spectrometer. When the line spacing is too large, the fine structures in the spectrum cannot be accurately measured, thus reducing the resolution. Secondly, the resolution of the grating spectrometer is also limited by the bandwidth of the light source and the geometry of the incident beam. If the bandwidth of the light source is large or the Angle of the incident beam changes greatly, the spectral line width resolved by the grating spectrometer will increase and the resolution will decrease accordingly.

In the future, there are several directions that can improve the resolution of the grating spectrometer. First, we need to improved raster technology can improve resolution. The manufacture of more precise gratings, including the use of advanced micro and nano machining techniques, can reduce the line spacing and improve the resolution. Then, the use of more broadband light sources and higher quality optical components, as well as the optimization of the grating spectrometer design, can reduce the geometric limit of the incident beam and improve the resolution. For example, the use of more advanced laser light sources and optimized optical design can reduce the bandwidth of the light source and thus improve the resolution. In addition, the introduction of advanced signal processing technology and data processing algorithm is also an effective way to improve the resolution of the grating spectrometer. Through the use of high-performance digital signal processors and advanced algorithms, spectral information can be extracted more accurately, further improving the resolution. Overall, the future direction of development includes improvements in grating technology, optimization of optical components and light sources, and innovation in signal processing technology, which will help improve the resolution of grating spectrometers. The realization of these visions requires interdisciplinary research and technological innovation, including further developments in the fields of optical engineering, nanotechnology, materials science, and computational science.

5. Conclusion

To sum up, the development history of grating spectrometer is summarized, and the structure and working principle of grating spectrometer are introduced in this paper. It involves indicators that affect its resolution. This study studies the ability of the grating spectrometer in different bands, and discusses the ability of the different band resolution and application differences to resolve the micro spectral characteristics. In areas where high scores are demanding, such as gas analysis and astronomical observations, higher resolution may be more advantageous. In the grating spectrometer, special attention should be given to the design of optical components, the stability of instruments and the impact of environmental factors. Future research can further focus on the technical improvement of the grating spectrometer to accommodate the application requirements of different bands.

Author Contribution

All the authors contributed equally and their names were listed in alphabetical order.

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