A new spectrometer using multiple gratings with a two-dimensional charge-coupled diode array detector

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Abstract
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Keywords
Ames Laboratory, Charge coupled devices, Image sensors, Diffraction gratings, Grating spectrometers, Silicon detectors

Disciplines
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Comments

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Charge-coupled devices as particle tracking detectors

A simple, low-cost, versatile charge-coupled device spectrometer for plasma spectroscopy
A new spectrometer using multiple gratings with a two-dimensional charge-coupled diode array detector

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A new spectrometer with no moving parts uses a two-dimensional Si-based charge-coupled diode (CCD) array detector and an integrated grating consisting of three subgratings. The effective spectral range imaged on the detector is magnified threefold. The digitized spectral image in the 200–1000 nm wavelength range can be measured quickly. The nonlinear relationship between CCD pixel position and wavelength is corrected with multiple polynomial functions in the calibration procedure, which fits the data using a mathematical pattern-analysis method. The instrument can be applied for rapid spectroscopic data analyses in many types of photoelectronic experiments and routine testing. © 2003 American Institute of Physics. [DOI: 10.1063/1.1573744]

I. INTRODUCTION

In the modern information age, it has become very important to acquire data rapidly, especially in the optical communication field where high-speed spectral analysis is needed.1 Usually, an optical dispersion system, such as a monochromator, is used in experiments.2 The optical dispersion element, a grating or prism, will be mechanically rotated continuously or in very fine steps to scan the wavelength and achieve high spectral resolution in the measurement. Usually it will take at least a minute or so to complete the wavelength scanning in the entire working spectral range due to the mechanical control process. For quick analysis of the spectrum with high resolution, several methods have been developed and studied.3,4 Instead of using a photomultiplier tube or a photon detector to detect the photons emerging from the narrow slit of the monochromator, a charge-coupled diode (CCD) array detector can be placed at the focal plane of spectral output of the monochromator with fixed mechanical and optical elements.5,6 The CCD array detector can record many spectral lines at its focal plane in a very short time. Because of several effects, however, the measurement will be restricted to a relatively narrow spectral range in applications. For example, at the focal plane of a monochromator with a typical dispersion of about 2 nm/mm, the effective wavelength measurement window is only about 48 nm for a CCD detector that has a photon-sensing area of about 24×24 mm² (total 1024×1024 pixels) with a 14–16-bit dynamical signal range in a typical application.7 In the near-ultraviolet-infrared range, the best Si-based CCD detector can be used to detect optical signals in the 200–1000 nm wavelength range. In order to take full advantage of the Si–CCD detector to cover the entire spectral range, mechanically scanning the wavelength window in many individual steps is still required.5,7 This window scanning process will significantly reduce the measurement speed and make operation less efficient and reliable.

In this work, we have improved the method by using a CCD array detector to measure the optical signal in the entire spectral range without scanning the wavelength window during the operation. Instead of using a single grating to diffract the light, a three-grating structure, which has different groove spacings and blaze wavelengths for each grating, was demonstrated in the design. The light diffracted by these three plane gratings will form a folded spectrum, which is imaged on the two-dimensional focal plane of the CCD detector. By careful design of the system, the optical spectral measurements can be completed in the 200–1000 nm wavelength range with high resolution at high speed, i.e., in less than 0.1 s. We will describe the method and performance in the following.

II. PRINCIPLE

For a plane grating (Fig. 1) with \( i \) and \( \theta \) the incidence and diffraction angles of light, respectively, with respect to the surface normal of the grating, diffracted quasimonochromatic light with wavelength \( \lambda \) in the \( n \)th order will be given by

\[
d(\sin \theta \pm \sin i) = m \lambda, \tag{1}
\]

where \( d \) is the distance between adjacent grooves on the grating surface. In the equation, a positive sign indicates that \( \theta \) and \( i \) are located on the same side of the surface normal, otherwise the sign will be negative. In the design, we use the negative sign because \( \theta \) and \( i \) are on opposite sides of the surface normal. By considering first-order (\( m = 1 \)) diffraction, Eq. (1) can be rewritten as

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\[
\sin \theta = m \lambda / d + \sin i = \lambda / d + g_0, \tag{2}
\]
where \(g_0\) is a constant related only to the incidence angle \(i\) of the light on the grating. For a fixed \(d\), the diffracted spectral lines will be distributed in a wavelength window \(\Delta \lambda\) corresponding to the diffraction angles ranging from \(\theta_1\) to \(\theta_2\):

\[
\sin \theta_2 - \sin \theta_1 = (\lambda_2 - \lambda_1) / d = \Delta \lambda / d. \tag{3}
\]

The spectral resolving power \(R\) in first order is defined as

\[
R = \lambda / \Delta \lambda = N, \tag{4}
\]
where \(N\) is the total number of grooves on the grating. For a typical grating with a groove density of 1200 g/mm and a useful width of 30 mm, \(R = 36,000\), which will give an ideal wavelength resolution of \(\Delta \lambda = 0.013\) nm at \(\lambda = 500\) nm. In practical applications, the resolution may not be as high as is expected. To get a rapid spectral measurement by using a CCD array detector, a large number of pixels may be required to cover the entire spectral range with high resolution. For example, in the 200–1000 nm wavelength range, at least 9000 pixels along the spectrum are needed to obtain a resolution of 0.1 nm for each pixel with the required minimum area size to produce enough photoelectrons in a high-dynamical 12–16-bit A/D signal-converting range. For a CCD detector with a standard 24×24 \(\mu\)m\(^2\) pixel size, the required total signal-sensing area will be 216 mm long. This is technically unrealistic for CCD design and fabrication. By taking the advantage of a two-dimensional CCD array detector, however, we can solve the problem of folding the spectrum in space. According to Eq. (3), for example, by taking proper grating \(d\) values, diffracted light with different wavelengths will be distributed in the same range of diffraction angles, i.e.,

\[
\Delta (\sin \theta) = \sin \theta_2 - \sin \theta_1 = (\lambda_4 - \lambda_3) / d_3 = (\lambda_3 - \lambda_2) / d_2 = (\lambda_2 - \lambda_1) / d_1. \tag{5}
\]

For example, three gratings with groove densities of 1200 g/mm \((d_1 = 833\) nm\), 600 g/mm \((d_2 = 1667\) nm\), and 300 g/mm \((d_3 = 3333\) nm\), respectively, can be used. Therefore, we have three wavelength windows, i.e.,

\[
\Delta \lambda_1 = \lambda_2 - \lambda_1 = 300 - 150 = 150\) nm, \tag{6}
\]
\[
\Delta \lambda_2 = \lambda_3 - \lambda_2 = 600 - 300 = 300\) nm, \tag{7}
\]
\[
\Delta \lambda_3 = \lambda_4 - \lambda_3 = 1200 - 600 = 600\) nm. \tag{8}
\]

The three windows can be arranged properly in two-dimensional space to cover the entire 150–1200 nm wavelength range in the same diffraction-angle range due to the constant ratios of \(\Delta \lambda_1 / d_1 = \Delta \lambda_2 / d_2 = \Delta \lambda_3 / d_3\). As seen in Fig. 2(a), the three gratings (each has dimensions of \(L/3 \times L\)), can be put together to form a new plane grating with the total grating size of \(L \times L\). In terms of a proper design of the optical system, three spectral-image zones corresponding to the three wavelength windows can be formed on the focal plane of the CCD array detector. The focal plane, consisting of 1024×1024 pixels, for example, will be divided into three spectral image zones. Each zone will have about 340×1024 pixels. Therefore, the effective measurement area along the wavelength direction will be magnified by three times in the space and will actually have about 3000 pixels in the 150–1200 nm wavelength range to measure the spectral lines. The average wavelength-to-pixel ratio in the three wavelength

![FIG. 1. Plane blazed grating.](Image)

![FIG. 2. (a) Three-grating structure, groove densities of (1) 1200 g/mm, (2) 600 g/mm, (3) 300 g/mm. (b) Optical configuration of the system.](Image)
windows of $\Delta \lambda_1$, $\Delta \lambda_2$, and $\Delta \lambda_3$ along the pixel direction, will be about 0.15, 0.3, and 0.6 nm/pixel, respectively. The principle given in this work also can be applied to a grating that can be designed and constructed with more subgratings having different groove $d$ values in order to get higher spectral resolution in applications.

III. EXPERIMENT

To test the principle of the method as mentioned earlier, we have used three plane subgratings with groove densities of 1200 g/mm (blazed at 860 nm), 600 g/mm (blazed at 400 nm), and 300 g/mm (blazed at 250 nm), respectively, to make an integrated plane grating in the experiment. The dimensions of each subgrating are $30 \times 10$ mm$^2$ with the grooves parallel to the short side. The total area of the integrated grating is $30 \times 30$ mm$^2$. The designed optical experiment system is shown in Fig. 2(b).

Light enters the slit having a fixed width of 0.04 mm and is reflected by mirror $M_1$ (focal length 110 mm). The parallel light from mirror $M_1$ is incident on the grating at incidence angle $i$, about 14.4°. In the incidence plane, the first-order diffracted light in the three wavelength windows, corresponding to the three subgratings with different groove $d$ values, is distributed in three zones with the same diffraction angles, as indicated by Eq. (5). According to Eqs. (1) and (5), this diffraction light window ($\Delta \theta = \theta_2 - \theta_1$) is equal to about 12.1°. The spectrum of the quasimonochromatic light is divided into three parts along the direction perpendicular to the incidence plane. For the subgratings arranged as shown in Fig. 2(a), those in the upper, middle, and low positions will diffract toward mirror $M_2$ quasimonochromatic light distributed in the 150–300, 300–600, and 600–1200 nm wavelength ranges with dispersions of about 7.5, 15, and 30 nm/mm, respectively. Toroidal mirror $M_2$, with the same focal length as $M_1$, in the direction parallel to the incidence plane, is used to reflect and form the spectral image on the focal plane of the CCD array detector. In the direction perpendicular to the incidence plane, the focal length of $M_2$ is about 550 mm. An advanced Apogee AP6 (UV) camera with a two-dimensional Si-based CCD array detector was used. The CCD detector has 1024×1024 pixels with a pixel size of 24×24 µm$^2$. Therefore, the total photoelectron sensing area is equal to about 25×25 mm$^2$ and has a 14-bit A/D signal converting capability. The speed for measuring the optical signal in the entire spectral range can be adjusted and controlled by the camera shutter through software according to the signal intensity. The minimum time for capturing a full frame of the spectral image on the focal plane of the CCD detector will be 0.01 s. Two high-pass filters with wavelength-cut edges at 300 and 580 nm were placed in front of the two subgratings (600 and 300 g/mm, respectively) to cut off second-order diffracted light. After taking a spectral image, the digitized spectral data were transferred immediately from the camera to the computer, saved, and were analyzed further in the experiment.

IV. RESULTS AND DISCUSSION

The typical spectral lines of a Hg lamp were measured by the system. An image of these spectral lines taken by the CCD camera is shown in Fig. 3. It can be seen clearly that there are three sub spectral regions in its image window corresponding to the three subgratings with different groove $d$ values. From left to right in Fig. 3, the wavelength is distributed in the 600–1200, 300–600, and 150–300 nm ranges, respectively. For the Si-based detector used in this instrument, wavelengths below 200 nm and above 1000 nm will not be measured. Due to imperfections in optical components, and also according to Eqs. (1)–(5), pixel position is not linear in wavelength in the two-dimensional image space. By using a mathematical pattern analysis method, therefore, multiple mathematical polynomial functions have been used to fit the spectral lines to the pixel positions in those three sub-spectral regions. For the best fitting to the data, the wavelength $\lambda$ is the function of the pixel position $x$ in the subwavelength region as

$$\lambda(x) = a_0 + a_1x + a_2x^2 + a_3x^3. \quad (6)$$

The advantage using the two-dimensional CCD array detector is that we can do spectral calibration on every pixel. As mentioned earlier, in each subregion of the CCD focal plane, there are $340 \times 1024$ pixels. This implies that there are 340 spectral lines, i.e., $\lambda(x)_1, \lambda(x)_2, \ldots, \lambda(x)_{340}$ along the direction parallel to the incidence plane with different sets of coefficient $a_n (n=0,1,2,3)$ according to Eq. (6). We can individually calibrate each such line, and then take the average of the line intensity $I(\lambda)$ with the same wavelength by adding them to increase the data accuracy. To avoid the error, a small part of data in the cross subspectral region was discarded. The calibrated spectral curves are shown in Fig. 4(a). Afterwards, the polynomial functions of the fitting curve, as shown in Fig. 5, were saved in the program and used in the experiment. The comparison between the measured and standard spectral lines of the Hg lamp is shown in Figs. 4(a) and 4(b).

The entrance slit with fixed width of 0.04 mm will be imaged with the same width showing on the focal plane of
better than 1.0 nm and agrees well with design expectations. The principle and method given in this work can be applied to optical systems with longer focal lengths and more sub-gratings to achieve higher spectral resolution.

The method studied in this work has been applied to a spectroscopic ellipsometric system in which the polarizer and analyzer are rotated and fixed, respectively. The elliptically polarized light containing the optical information from the sample passes through the fixed analyzer and then enters the spectrometer system with the CCD array camera as designed in this work. Instead of mechanically scanning the wavelength in each operation step, the spectral data in the entire wavelength range at each azimuth angle of the polarizer can be measured in less than 0.1 s with good signal-to-noise ratio. The complex dielectric function of a gold sample was measured, for example, showing results in good agreement with those measured by other methods. We will discuss the method in more detail elsewhere.

In this work, we have designed a new type of spectrometer system by using a two-dimensional Si-based CCD array detector and an integrated grating consisting of three sub-gratings. The effective spectral area for measuring spectral data in the limited focal plane of the detector is magnified by a factor of 3. The digitized spectral image in the 200–1000 nm wavelength range can be quickly measured without any mechanical moving part in the system. The nonlinear relationship between the CCD pixel position and wavelength has been studied with multiple polynomial functions in the calibration procedure to fit the data by using the mathematical pattern analysis method. The principle can be applied to systems for doing rapid spectroscopic data analysis in many types of photoelectronic experimental research.

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