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Calculation of the diffraction efficiency on concave gratings based on Fresnel–Kirchhoff's diffraction formula

Yuanshen Huang,^{1,*} Ting Li,¹ Banglian Xu,¹ Ruijin Hong,¹ Chunxian Tao,¹ Jinzhong Ling,¹ Baicheng Li,¹ Dawei Zhang,^{1,2} Zhengji Ni,¹ and Songlin Zhuang¹

¹Engineering Research Center of Optical Instrument and System, Ministry of Education and Shanghai Key Laboratory of Modern Optical Systems, University of Shanghai for Science and Technology, No. 516 JunGong Road, Shanghai 200093, China

²School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

*Corresponding author: hyshyq@sina.com

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Fraunhofer diffraction formula cannot be applied to calculate the diffraction wave energy distribution of concave gratings like plane gratings because their grooves are distributed on a concave spherical surface. In this paper, a method based on the Kirchhoff diffraction theory is proposed to calculate the diffraction efficiency on concave gratings by considering the curvature of the whole concave spherical surface. According to this approach, each groove surface is divided into several limited small planes, on which the Kirchhoff diffraction field distribution is calculated, and then the diffraction field of whole concave grating can be obtained by superimposition. Formulas to calculate the diffraction efficiency of Rowland-type and flat-field concave gratings are deduced from practical applications. Experimental results showed strong agreement with theoretical computations. With the proposed method, light energy can be optimized to the expected diffraction wave range while implementing aberration-corrected design of concave gratings, particularly for the concave blazed gratings. © 2013 Optical Society of America

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1. Introduction

Concave gratings play an important role in spectroscopy field since they integrate the functionality of dispersion and focus together. In most cases high resolution is a quite important indicator to evaluate the performance of gratings, but it is not the unique criterion, especially in the situation of weak spectral energy, more attention should be paid to concentrate the diffraction light energy on the specific wavelength range. Therefore, calculation for the energy distribution of the diffraction field is also a significant task. The theoretical system for plane gratings

was established based on the Fraunhofer diffraction theory. Born and Wolf [1] calculated the diffraction efficiency of a plane grating by solving the transmission field of multiple slits. As for many different kinds of plane gratings, blazed grating is regarded as a vital one because its diffraction energy can be concentrated near an expected wavelength just by changing the angle of groove surfaces, which is described in detail by Hutley [2] for both transmission and reflection plane blazed gratings. For a more accurate calculation, the groove patterns and material properties of gratings must be considered. Combine with the boundary condition of grating, diffraction fields of transverse electric and transverse magnetic polarization are first obtained by solving the Maxwell's equations, after which the diffraction

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efficiency is computed [3]. Moharam and Gaylord proposed the rigorous coupled-wave theory and set up the theoretical model on calculating diffraction efficiency of one-dimensional rectangular gratings [4]. This theory was developed for suiting arbitrary grating groove profile later [5–8]. The above-mentioned theories are just fit for plane gratings with equidistant and straight grooves. Although the concave grating was first introduced by Rowland as early as 1882 [9], only a few studies on the calculation of its diffraction efficiency were reported. One reason is that grooves of a concave grating are distributed on a concave substrate, wherein the Fraunhofer diffraction equation cannot be used. Moreover, if vector diffraction theory is selected, the two-dimensional groove surfaces must be divided into a finite number of small units, and then the diffraction field on each unit is calculated with considering the boundary condition among adjacent units. Obviously the more units we divided, the more accurate result can be got, but the data volume is becoming larger at the same time, which means a more complex computation. Another reason is that in the concave grating application, the incident wave is divergent spherical wave emitted by point light source and becomes convergent after the grating diffraction. Therefore, the positions of both source and receiving surface have to be considered simultaneously in the diffraction efficiency calculation, which will also increase the difficulty of the process. At present, most fabricants and users of concave gratings generally use the actual measuring instruments to obtain the diffraction efficiency. As a result, diffraction energy cannot be designed to concentrate in the specific wavelength range before manufacturing, which will cause a waste of resource and time.

Few studies have been published about the diffraction efficiency of concave gratings. Hunter and co-workers [10,11] reported the differences of diffraction efficiency between holographic lithography grating and mechanical ruled grating based on theoretical calculations and experimental results. But the authors adopted plane grating model for approximation due to the small curvature of the selective concave grating. Bazhanov and Kulakova [12] established the functional relation between grooves at arbitrary position and the apex of the concave grating. Analytic expressions of diffraction energy distribution were derived by utilizing the geometrical relation between incident rays of arbitrary grooves and principle one. Kulakova *et al.* [13] set up the mathematic model on a concave grating when the spherical wave was incident. The analysis on the distribution as well as variable spacing of grooves was added, and then the diffraction efficiency distribution in the principal section was discussed by both the scalar and vector method. Ko *et al.* [14] first discovered the double-reflection phenomenon of the concave blazed grating and simulated the diffraction efficiency of Rowland-type concave grating by PCGrate software.

However, all the calculation models on diffraction efficiency discussed above were established in the principal section of a concave grating, which ignored the influence of the nonprincipal section. This presupposition will cause large errors when the grating curvature is big. An ideal calculation model should consider the influence of the entire concave surface on the diffraction efficiency. According to this thought, a calculation model on the concave grating with sawtooth grooves is going to be established under spherical wave incidence. The whole procedure can be described as three main steps: first, an arbitrary grating groove was divided into finite diffraction apertures and the diffraction complex amplitude on each aperture was calculated based on the Fresnel–Kirchhoff's diffraction formula. Then the total complex amplitude of the whole concave grating is got by superimposing the results from all apertures of every groove. Finally, the diffraction efficiency of a concave grating is obtained by a simple transformation from the complex amplitude. In this article, the relationship between the diffraction efficiency of a Rowland-type concave grating and different parameters, i.e., incident angle, F number, number of grooves, is analyzed, respectively. The calculation method of diffraction efficiency for a flat-field concave grating is illustrated, and the peak variations are compared among different usage conditions. Experimental results are also given in the end, which show basically coincident with the theoretical computation, and hence the proposed method will provide some certain reference values to the design and fabrication of a concave grating.

2. Principle

Supposing grooves of a concave grating are formed on the reflective coating that is deposited on the concave substrate. Due to mechanical ruling with a diamond graver is a commonly used manufacturing way, groove shapes are sawtooth with a definite angle or triangular which is consistent with the cutter edge of graver. Generally, all grooves are parallel and distributed along a certain orientation, so the projections on the tangent plane of the grating vertex are straight lines that are either equidistant or nonequidistant. According to different operating conditions, the grating grooves can also be equidistant or nonequidistant curves after carrying out aberration-corrected design. In this article we focus on the former situation.

A. Rowland-Type Concave Grating

If the incident slit is set on the Rowland circle, the diffraction image will focus automatically on the same circle [9]. Sharp spectral lines can be obtained in this situation since the meridional astigmatic is zero on the Rowland circle. This kind of device has wide applications due to its simple structure and convenient adjustment.

As shown in Fig. 1, first we assume the N pieces of sawtooth grooves are equidistant and parallel to

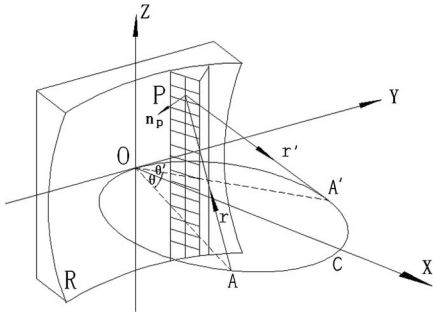


Fig. 1. Structure of Rowland-type concave grating.

each other. A coordinate system is set up with the origin at the vertex $O(0, 0, 0)$ of the concave grating, X axis points to the normal direction at vertex while Z axis parallels to the tangential direction of grooves. Grating substrate is a spherical surface with curvature radius R , and its center is at $C(0, 0, R)$. In the principal section (XOY plane), a spherical wave emitted from $A(r \cos \theta, -r \sin \theta, 0)$ is diffracted when encountering an arbitrary point $P(x, y, z)$ on any groove surface, and the image point for a certain wavelength will be focused on $A'(r' \cos \theta', r' \sin \theta', 0)$, which lies on the Rowland circle too. According to the characteristic of fabrication, each groove surface is a cone surface rotating about a certain rotor, with the diamond blade used as generatrix. Different groove faces have different rotating shafts, but they are all parallel to the Y axis and the distance from them to the bottom of their corresponding groove is equal to R . Therefore, grating profiles ruled in this way are parallel straight grooves.

As point $P(x, y, z)$ located on the spherical surface, its coordinate values must satisfy the spherical equation

$$(x - R)^2 + y^2 + z^2 = R^2. \quad (1)$$

Then since principal rays meet the grating equation, which can be denoted by

$$\sin \theta - \sin \theta' = \frac{1}{e_0} k \lambda, \quad (2)$$

where e_0 is the grating constant at vertex O , k is the diffraction order, λ is the diffraction wavelength, θ and θ' are the incident and diffraction angles, respectively. Each groove face is equally divided into n pieces of small diffraction units, each of which can be considered approximately as a small plane. The dimension of these small planes is larger than wavelength, but much smaller than the distance from A or A' to points on these diffraction units. Assuming n_p represents the normal vector of a small plane at point P , so the Fresnel–Kirchhoff's diffraction formula corresponding to this plane can be expressed as

$$\begin{aligned} \tilde{E}_i(A') = & \frac{B}{i\lambda} \iint_{\Sigma} \frac{\exp(ikr)}{r} \frac{\exp(ikr')}{r'} \\ & \times \left[\frac{\cos(n_p, r) - \cos(n_p, r')}{2} \right] d\sigma, \quad (3) \end{aligned}$$

where

$$r = |AP| = [(x - r \cos \theta)^2 + (y - r \sin \theta)^2 + z^2]^{\frac{1}{2}}, \quad (4)$$

$$r' = |A'P| = [(x - r' \cos \theta')^2 + (y - r' \sin \theta')^2 + z^2]^{\frac{1}{2}}, \quad (5)$$

$$\cos(n_p, r) = \frac{\vec{n}_p \cdot \vec{r}}{|\vec{n}_p| \cdot |\vec{r}|}, \quad (6)$$

$$\cos(n_p, r') = \frac{\vec{n}_p \cdot \vec{r}'}{|\vec{n}_p| \cdot |\vec{r}'|}. \quad (7)$$

As shown in Fig. 2, α is the angle between groove surface at vertex O and Y axis, then the normal vector n_p is got by using space analytic geometry

$$\vec{n}_p \left(-\cos \alpha \frac{R-x}{zR}, \sin \alpha \cos \theta \frac{R-x}{zR} + \frac{\sin \alpha \sin \theta}{R}, \frac{\cos \alpha}{R} \right). \quad (8)$$

Assuming that the grating width and height are W and H , respectively, then the grating constant e_0 for equidistant grating can be written as: $e_0 = w/N$, and the height of each small diffraction unit is H/n . Obviously, the larger the n chosen, the more accurate the calculation results will be. The complex amplitude of a single groove at point A' can be expressed as follows:

$$\tilde{E}_j(A') = \sum_{i=1}^n \tilde{E}_i(A'). \quad (9)$$

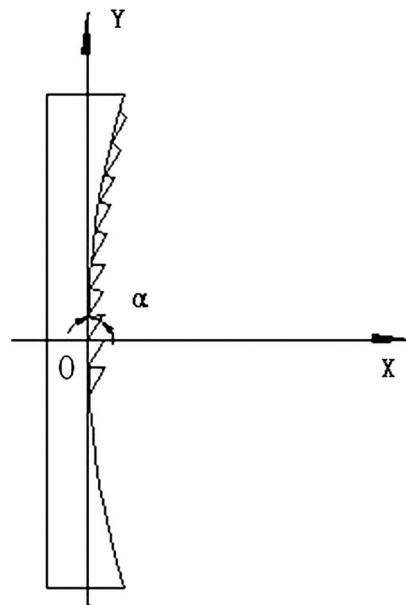


Fig. 2. Principal section of concave grating.

Then the total complex amplitude at point A' for the whole N pieces of groove can be written as

$$\tilde{E}(A') = \sum_{j=1}^N \tilde{E}_j(A'). \quad (10)$$

The diffraction field distribution of Rowland-type concave gratings can be calculated by Eqs. (1)–(10). At a certain order, the light intensity distribution for different wavelengths can be obtained by squaring the relevant total complex amplitude, which provides significant reference values to the design of concave grating with high resolution and reasonable energy distribution.

B. Flat-Field Concave Grating

With the extensive applications of linear and area-array detectors, optical spectrum instruments are developed to the direction of miniaturization, high-speed, and simultaneous multichannel detection. These instruments need to focus the detected spectrums onto a plane. In this case, flat-field concave grating is considered as an ideal spectral component which can disperse the incident light in one plane after aberration-corrected design and precision grating fabrication. For a flat-field concave grating with given incident slit and image position, if we take an astigmatism-corrected design for the most significant astigmatism, the grating grooves will change into nonequidistant parallel straight lines, and its distribution function is defined as

$$y + \frac{1}{2}u_{20}y^2 = e_0m, \quad (11)$$

where $m = 0, \pm 1, \pm 2, \dots$, e_0 is the effective grating constant at the grating vertex, and u_{20} is a constant getting from the astigmatism-corrected calculation [15,16].

Figure 3 shows the schematic diagram of the flat-field concave grating, where A is the midpoint of incident slit, A' is a diffraction image focused on the plane L for a certain wavelength, and r' is the distance from an arbitrary point P of grooves to the image point on the plane L . The method of calculating the diffraction efficiency is the same as that discussed in Subsection 2.A, except that the grooves

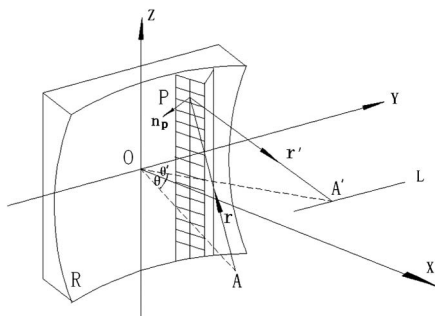


Fig. 3. Structure of flat-field concave grating.

are no longer equidistant. The distribution of grating grooves must be calculated first by Eq. (11) and then combined with Eqs. (3) and (10) to obtain the final result.

3. Simulation and Experiments

A. Software Simulation by Matlab

According to the theoretical model presented above, we simulated the diffraction efficiencies of Rowland-type and flat-field concave gratings with sawtooth grooves at visible wavelengths (400–700 nm). The influence of several parameters, like incident angle, F number, and number of grooves on diffraction efficiency, is discussed separately.

1. Effects of Incident Angle on Diffraction Efficiency

Figure 4 shows the +1st-order diffraction efficiency curves of Rowland-type concave grating, which varies with wavelength at different incident angles. The grating grooves are parallel and equidistant with a density of 600 g/mm, the angles of their surfaces are all equal to 10° . Grating substrate size is 10 mm \times 10 mm. The selected incident angles are 6° , 8° , and 10° .

As we can see from Fig. 4, the peak of diffraction efficiency shifts to the longer wavelength as the incident angle gradually increases. According to this regulation, maximum diffraction efficiency can be optimized to the necessary spectrum range by adjusting the incident angle, which will greatly increase the utilization of energy.

2. Effects of F Number on Diffraction Efficiency

F number is one of the most important factors that influence the diffraction efficiency. It is defined by f/d for gratings, where f is the focal length and d is the clear aperture of gratings. Once the grating aperture size is determined, a short curvature radius will correspond to a small F number. Figure 5 shows the +1st-order diffraction efficiency curves of

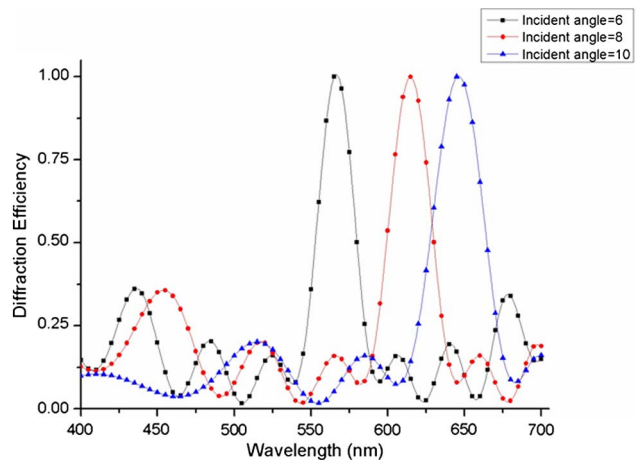


Fig. 4. (Color online) Diffraction efficiency versus wavelength at different incident angles.

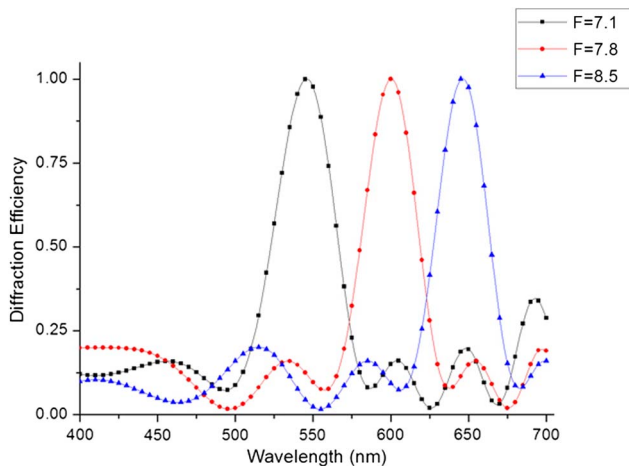


Fig. 5. (Color online) Diffraction efficiency versus wavelength at different F numbers with incident angle equal to 10° .

Roland-type concave grating, which varies with wavelength at different F numbers. The grating grooves are parallel and equidistant with a density of 600 g/mm , both incident angle and groove surface angle are 10° . Grating substrate size is $10\text{ mm} \times 10\text{ mm}$. The chosen F numbers are 7.1, 7.8, and 8.5.

According to Fig. 5, the peak of diffraction efficiency shifts to the longer wavelength as the F number gradually increases. With this regulation, energy on the expected spectral range can be optimized during the course of aberration-corrected design. Higher diffraction efficiency as well as optimization for resolution and dispersion can be obtained by changing the F number.

3. Effects of Number of Grating Grooves on Diffraction Efficiency

For the concave grating, the usage spectrum range, dispersion, and resolution are partly determined by the total number of grating grooves. Moreover, diffraction efficiency will also be affected by the density of grating grooves for a specified spectral range. Figure 6 shows the +1st-order diffraction efficiency curves of Roland-type concave grating, which varies with wavelength at different densities of grating grooves. The grating grooves are parallel and equidistant, both incident angle and groove surface angle are 10° . Grating substrate size is $10\text{ mm} \times 10\text{ mm}$. The densities of grating grooves are 600 g/mm , 650 g/mm , and 700 g/mm .

From Fig. 6, we can see that the peak of diffraction efficiency shifts toward the shorter wavelength as the densities of grating grooves gradually decrease, which provide some definite reference values to the design of the concave grating.

For the situations discussed in Figs. 5 and 6, if the incident angle is reduced from 10° to 6° , then the peak position of diffraction efficiency will all shift to the shorter wavelength. This is corresponding to the conclusion given in Fig. 4. Besides the bandwidth of each curve becomes relatively narrower. The simulation results are shown in Figs. 7 and 8, respectively.

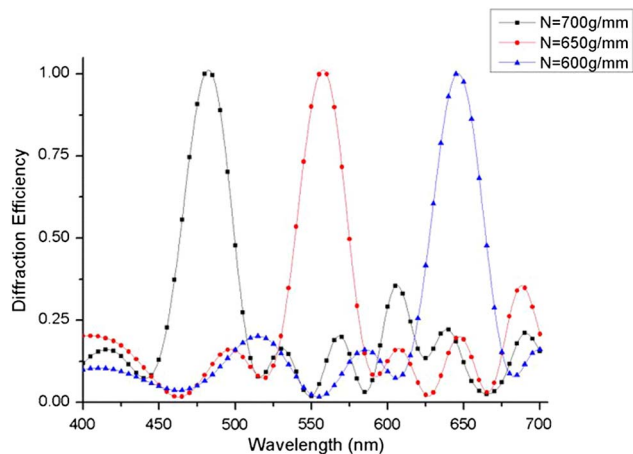


Fig. 6. (Color online) Diffraction efficiency versus wavelength at different densities of grating grooves with incident angle equal to 10° .

It can be deduced that if the F number or density of grating grooves is determined, a decrease in incident angle will cause the peak position to shift to the shorter wavelength and narrower bandwidth.

4. Diffraction Efficiency Curve of Flat-Field Concave Grating

The groove distribution function of aberration-corrected flat-field concave grating is dependent on the usage condition, such as spectrum range, density of grating groove, detector size on image plane, curvature radius of grating, and position of incident slit. Although the effects of those parameters on the calculation of diffraction efficiency are rather complex, the method introduced in Section 2 can obtain the diffraction efficiency of a given flat-field concave grating conveniently with the aid of software such as Matlab. Figure 9 shows the calculated result of the -1st order diffraction efficiency curve for a flat-field concave grating, where the curvature radius is 120 mm , both incident angle and groove surface angles are 10° , grating substrate size is

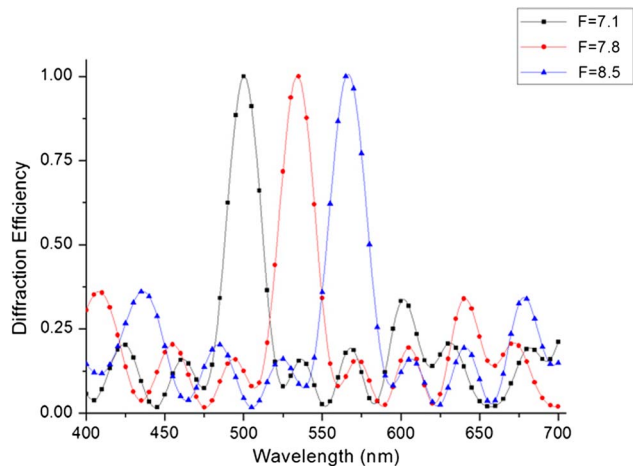


Fig. 7. (Color online) Diffraction efficiency versus wavelength at different F numbers with incident angle equal to 6° .

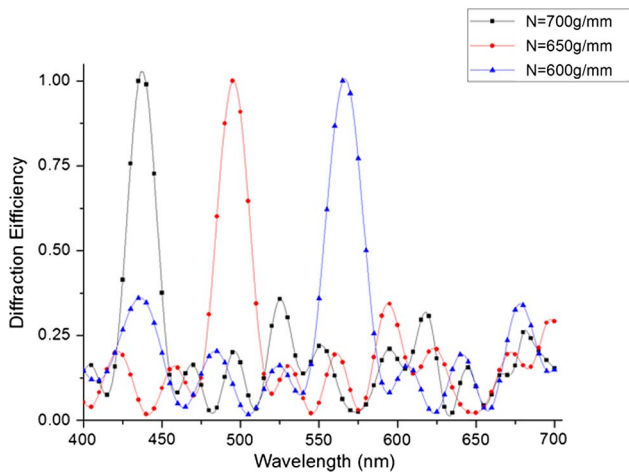


Fig. 8. (Color online) Diffraction efficiency versus wavelength at different densities of grating grooves with incident angle equal to 6° .

10 mm \times 10 mm, and density of grating grooves is 500 g/mm. The groove distribution function deduced from the given grating is written as

$$y + 0.5 \times 0.0056y^2 = e_0m, \quad (12)$$

where e_0 is the effective grating constant at vertex, $m = 0, \pm 1, \pm 2, \dots$

The peak of diffraction efficiency in Fig. 9 lies at about 450 nm. Using this method, the energy distribution can be acquired quickly while carrying out the optimization design of aberration. Moreover, flat-field concave gratings with high resolution and reasonable energy distribution can be obtained through repeated trials.

B. Experimental Result

A Rowland-type concave grating was designed and fabricated with the following parameters: curvature radius at 110 mm, density of grating grooves at 600 g/mm, both groove surface angle and incident angle at 10° , and grating substrate size at

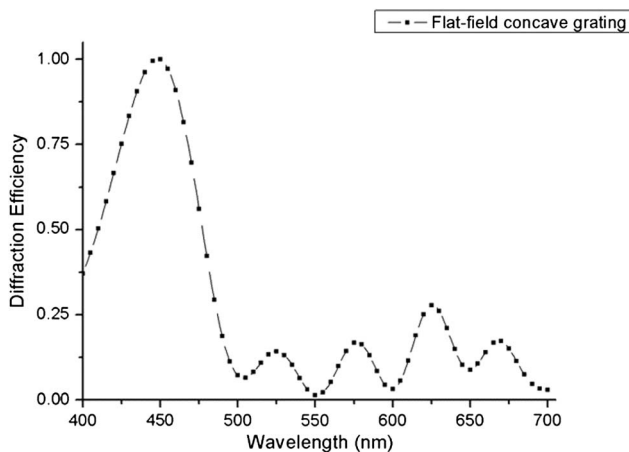


Fig. 9. Diffraction efficiency versus wavelength for flat-field concave grating.

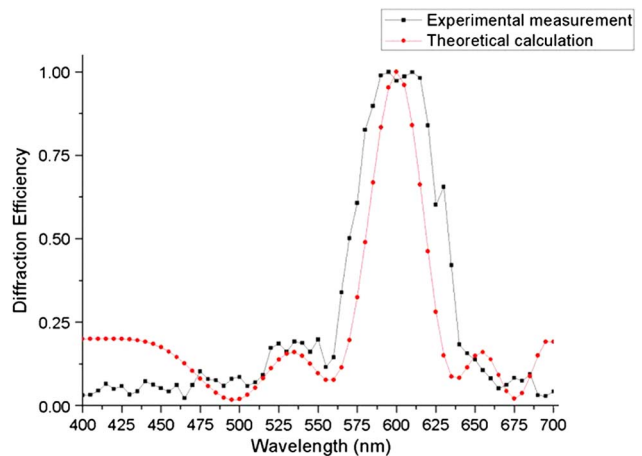


Fig. 10. (Color online) Diffraction efficiency curves of both theoretical calculation and experimental measurement for Rowland-type concave grating.

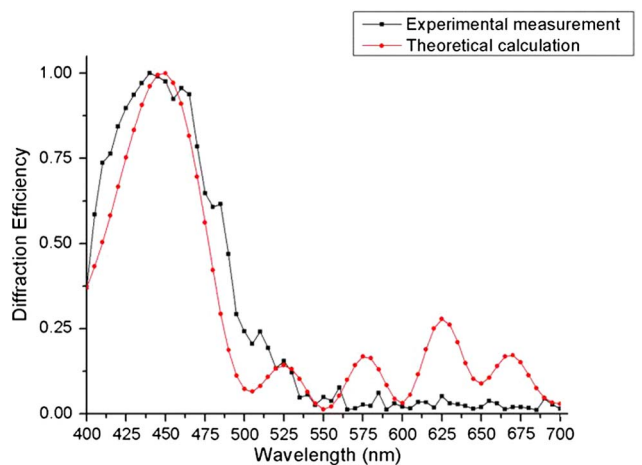


Fig. 11. (Color online) Diffraction efficiency curves of both theoretical calculation and experimental measurement for flat-field concave grating.

10 mm \times 10 mm. Figure 10 shows the diffraction efficiency curves of both practical measurement and theoretical calculation.

A flat-field concave grating was also designed and fabricated with the following parameters: curvature radius at 120 mm, density of grating grooves at 500 g/mm, both groove surface angle and incident angle at 10° , and grating substrate size at 10 mm \times 10 mm. Figure 11 shows the diffraction efficiency curves of both practical measurement and theoretical calculation.

As shown in Figs. 10 and 11, both curves in each figure appear as a similar trend. The noncoincidence between the theoretical and the practical result is caused by the approximation made in the theoretical analysis, fabrication as well as measurement errors, and so on.

4. Conclusion

We have successfully calculated the diffraction efficiency of concave gratings with sawtooth grooves

based on the Fresnel–Kirchhoff’s diffraction formula. This achievement fills a theoretical gap with taking the influence of grooves in nonprincipal section into consideration. The diffraction efficiency curves, which vary with wavelength at different parameters, such as incident angle, F number, and number of grating grooves, is also analyzed. The consistency between theoretical simulation by Matlab and practical measurement results illustrates that our proposed method is a new and useful approach to solve the diffraction efficiency on concave gratings. Using this calculation method, the distribution of diffraction efficiency with wavelength can be solved accurately and quickly while the design and usage parameters are given; therefore, the efficiency peak is easy to be optimized to the desired wavelength and the purpose of blazing will be achieved.

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