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An equivalent field principle and the multiple Kirchhoff integral method for UV blazed gratings

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Abstract

In order to solve the surface-shadowing problems that take place in the scattering of electromagnetic waves from rough or period surfaces, an equivalent field principle for plane waves scattering from plane surfaces is given in this paper. Supported by this principle, the reciprocity theorem, and the boundary conditions that relate the scattering field to the incident field through the Fresnel coefficient, a multiple Kirchhoff integral method for metal blazed gratings is developed. Under the conditions of Littrow mounting or fixed angular deviation mounting, illuminated by plane waves, the -1 order's and/or the total efficiencies of perfectly conducting or UV aluminum blazed gratings are calculated and the stability and the self-consistency of this method are discussed. Under near-Littrow mounting (the fixed angular deviation mounting but where the angular deviation is very small) conditions, the calculations are compared with the experimental results.

Keywords: Multiple Kirchhoff integral; Littrow mounting; Fixed angular deviation mounting; Reciprocity theorem; Equivalent field principle

1. Introduction

The anomalous behavior of diffraction gratings, which was first observed by Wood [1], has attracted a large number of theoretical and experimental researchers. Recently, more and more analysis of various diffraction gratings working in the UV, VUV or X-ray region has been reported [2–4]. However, most of this work is theoretically based on the mode-couple method, the integral method or the differential method explicated systematically by Petit [5].

Palmer and LeBrun [8] studied the efficiency problem and the anomalous behavior of perfectly conducting blazed gratings with the multiple Kirchhoff integral method first, since the early works of McPhedran [6] and Huntley [7] demonstrated that the single scalar Kirchhoff integral method was not self-consistent and could not explain the anomalies of gratings. The superior of the multiple Kirchhoff integral method is that we can avoid the problem of determining the accurate current distribution on the grating surface by following a suggestion by Stone [9]. However, they did not give more details such as the stability and the self-consistency of the method, perhaps because the calculation time of those prob-

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lems was too large for even the best computers at that time.

Today, fortunately, utilizing a general Pentium II PC of processor frequency 350 MHz, in this paper we could develop the multiple Kirchhoff integral method in the following respects:

Firstly, to extend the method to real metal gratings, Jackson's boundary conditions [10,11], which define the actual scattered or diffracted fields on the boundary to be the 'total field minus the incident field', are introduced.

Secondly, to solve the shadowing problems not solved by Palmer and LeBrun while dealing with blazed gratings, an equivalent field principle is given.

Thirdly, the stability and self-consistency of this developed multiple Kirchhoff integral method are discussed by means of the total efficiency calculations of perfectly conducting blazed gratings.

Fourthly, under the conditions of Littrow mounting or fixed angular deviation mounting, the -1 order's efficiencies of UV aluminum blazed gratings while incident waves are both S polarized (the magnetic field is parallel to the grooves) and P polarized (the electric field is parallel to the grooves) are calculated.

And lastly, to examine the reliability of the developed multiple Kirchhoff integral method, while the UV aluminum blazed gratings are shined by the unpolarized plane electromagnetic waves and under near Littrow mounting conditions, the calculated -1 order's efficiencies are compared with the experimental results [12].

2. Multiple Kirchhoff integral method

2.1. Basic theory

In our theory, the incident electromagnetic wave excites all of the spots on the facets of the blazed grating to be the second sources, and all of the second sources in one facet emit spherical waves to all of the spots in space or on the opposite facet. The amplitudes and the phases of the scattered waves are determined by the amplitudes and the phases of the incident waves, from the actual scattered fields boundary conditions that are approximated and defined by Jackson to be 'total field minus the incident field'. Also, the complex amplitudes of arbitrary spots in space are the vector sum of the scattered waves from all of the second sources. Such a method, taking into account only the effect of second sources or the first scattering, is the single Kirchhoff integral method.

However, the single Kirchhoff integral method cannot demonstrate the anomalous behavior of diffraction gratings [6], simply because of the neglect of the multiple scattering phenomena. In our theory, the vector sum of the scattered waves from second sources may excite the spots on the opposite facets of the blazed grating to be the third sources, and the third sources may excite the fourth sources, and so on. The complex amplitude of one spot in space is the vector sum of the waves from all of the sources, in all facets, and at all times. The theoretical analysis and the simulated calculation of Palmer and LeBrun [8] demonstrated that, without shadowing problem, the sum of the first three-times scattering may describe the anomalous behavior of the gratings and retain sufficient precision.

2.2. Boundary conditions

From wave optics, the scattering boundary conditions for random roughness surfaces may be used as the diffracting boundary conditions for period gratings. Also, the vector boundary conditions that relate the scattering fields to the incident fields have been given by Jackson [11] and Holzer and Sung [10]:

$$\vec{E}_{\rm s}^{\rm s} = -\vec{n}_r \times \gamma_{\rm s} \vec{B}_{\rm in}^{\rm s},\ \vec{B}_{\rm s}^{\rm s} = \gamma_{\rm s} \vec{B}_{\rm in}^{\rm s},\ \vec{E}_{\rm s}^{\rm p} = \gamma_{\rm p} \vec{E}_{\rm in}^{\rm p},$$
$$\vec{B}_{\rm s}^{\rm p} = \vec{n}_r \times \gamma_{\rm p} \vec{E}_{\rm in}^{\rm p}, \tag{1}$$

$\vec{n}_r = \vec{n}_0 - 2\vec{n}'(\vec{n}\cdot\vec{n}_0)$ and $\vec{n}'$ is the perpendicular of the grating facet, $\gamma_{\rm s}$, $\gamma_{\rm p}$, are the Fresnel reflection factor of S and P polarization and defined as:

$$\gamma_{\rm s} = \frac{\tan(\theta_{\rm i} - \theta_{\rm r})}{\tan(\theta_{\rm i} + \theta_{\rm r})} \quad \gamma_{\rm p} = -\frac{\sin(\theta_{\rm i} - \theta_{\rm r})}{\sin(\theta_{\rm i} + \theta_{\rm r})}, \tag{2}$$

$\theta_{\rm i}$ is the incident angle, $\theta_{\rm r}$ is the refraction angle, they are related by $\hat{n}_{12}\ \sin\theta_{\rm r} = \sin\theta_{\rm i}$, and $\hat{n}_{12} = n_{12} + {\rm i} k_{12}$ is the complex refracting power of the grating material.

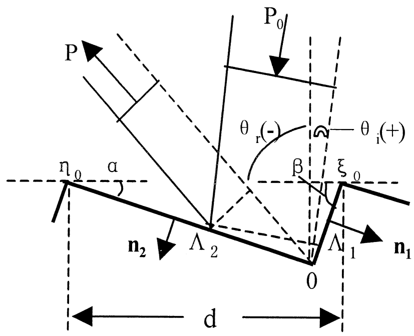

Fig. 1. Blazed grating groove geometry with ray incident from P_0 and diffracted to P.

2.3. Equivalent field principle

One groove of a blazed grating is shown in Fig. 1. The wideness of the groove is d, the antiblaze surface Λ_1 makes angle β with the grating surface, and the blaze surface Λ_2 makes angle α with the grating surface. The normal of Λ_1 or Λ_2 is $\vec{n}_1$ or $\vec{n}_2$, and the direction of incident or diffracted plane wave is P_0 or P.

The diffracting situations of blazed gratings discussed and calculated by Palmer and LeBrun [8] are only restricted to the condition of $a - \pi/2 < \theta_i$ and $\theta_r < \pi/2 - \beta$, i.e., the angles for which both source and detector can see all parts of the grating facet and there are no shadows involved.

In fact, all the diffracted gratings may be incident and diffracted in the angular range of $-\pi/2 < \theta_i$ and $\theta_r < \pi/2$. Thus, we cannot completely get any one efficiency curve of arbitrary order which satisfies the equation of blazed gratings:

$$\sin\theta_r = -\sin\theta_i - m\frac{\lambda}{d}, \tag{3}$$

not to say getting the total efficiency curve of an arbitrary blazed grating with any incident angle. If we want to discuss the self- consistency of this multiple Kirchhoff integral method, what we must do first is solve the shadowing problem in the course of diffraction. For this purpose, an equivalent field principle is described as follows.

Because the transverse dimensions of the facets of the gratings are comparable with the wavelength of the incident waves, while the gratings irradiated by plane electromagnetic waves and detected in the far field conditions, an equivalent field principle may be utilized to solve the shadowing problem:

As shown in Fig. 2, in vacuum, the complex amplitude of a free plane electromagnetic wave $E = A\exp(i(k_x \cdot x + k_y \cdot y))$ on the plane $y - lx + c = 0$ is equal to the complex amplitude of the plane electromagnetic wave $E_1 = A\exp(i(k_{1x} \cdot x + k_{1y} \cdot y))$ in this plane and

$$k = k_1, \quad \left(k = \sqrt{k_x^2 + k_y^2},\ k_1 = \sqrt{k_{1x}^2 + k_{1y}^2}\right), \tag{4}$$

$$\theta = \theta_1. \tag{5}$$

When a plane electromagnetic wave propagates freely in vacuum and does not encounter any mate-

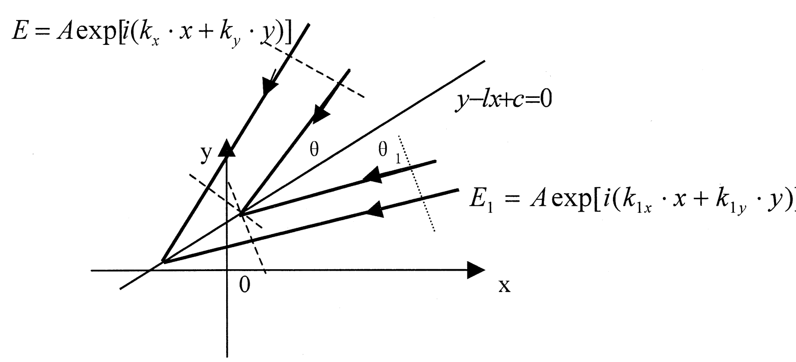

Fig. 2. The plane wave field E and its equivalent field E_1 on the plane $y - lx + c = 0$.

rial, there is no electromagnetic field scatted, and the scattered field may be defined as:

$$E_s = E - E_1 = E + (-E_1), \tag{6}$$

and its value is 0. We define $-E_1$ as E_e, the equivalent field of the incident plane wave field.

When a plane electromagnetic wave is scattered by an ideal conductor surface, the equivalent field defined as Eq. (6) is also equal to 0, only because it is inside the conductor. If the polarization of incident wave is taken into account, Eq. (6) may be rewritten as:

$$E_s = \pm(E + E_e). \tag{6'}$$

Under S polarization the positive sign is taken, and under P polarization the negative sign is taken.

When a plane electromagnetic wave is scattered by a real conductor or a non-transparent dielectric surface, if the transmission wave may be neglected, then the equivalent field is also 0. Thus, we may extend Jackson's vector boundary conditions [10,11], which define the actual scattered field to be the 'total field minus the incident field', and relate the scattered field to the incident field through the Fresnel coefficient, to be

$$\vec{E}_s^s = -\vec{n}_r \times \left[\gamma_s\left(\vec{B}_{in}^s + \vec{B}_{e,in}^s\right)\right],$$

$$\vec{B}_s^s = \gamma_s\left(\vec{B}_{in}^s + \vec{B}_{e,in}^s\right), \vec{E}_s^p = \gamma_p\left(\vec{E}_{in}^p + \vec{E}_{e,in}^p\right),$$

$$\vec{B}_s^p = \vec{n}_r \times \left[\gamma_p\left(\vec{E}_{in}^p + \vec{E}_{e,in}^p\right)\right]. \tag{7}$$

Because, in our discussion, the incident and the diffracted electromagnetic waves are all plane waves, we can estimate whether the incident field and/or the diffracted field exist by the geometrical optics criterion. An equivalent field principle for the substitution of plane wave field may be described as follows:

(1) When the incident field is projected onto a scattering facet without any shielding effect, the equivalent field is symmetrically distributed to the incident field about the scattering facet, so that the equivalent field is shielded to be 0 by the scattering body.

(2) When the incident angle, which is decided by the vector of incident field and the perpendicular of the facet, is larger than $\pi/2$, the incident field is shielded to be 0 by the scattering body, but the equivalent field exists. Thus, the effect of the incident field on the scattering facet may be substituted by the effect of its equivalent field.

(3) When the incident field is shielded by other conductor or non-transparent object, but not by the scattering facet itself, the incident field and its equivalent field are all equal to 0.

Supported by the equivalent field principle above, the reciprocity and the energy conservation principle, the developed multiple Kirchhoff integral method for blazed gratings can be discussed below.

2.4. Multiple Kirchhoff integral formulae

As shown in Fig. 3, taking account of the length of this paper and continuity of Palmer and LeBrun's work [8], in the following, involving the shadowing effect, we simply write out the complex amplitudes

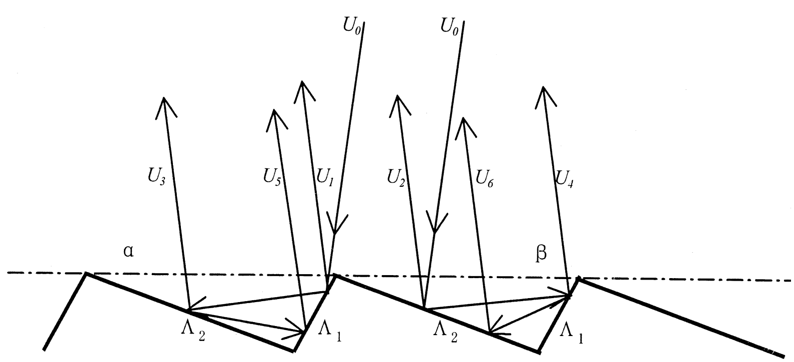

Fig. 3. Various multiple diffraction terms from the grating grooves. Incident field U_0 on Λ_1 at right gives rise to U_1, U_3 and U_5 (single, double, and triple diffractions). Incident field U_0 on Λ_2 at right gives rise to U_2, U_4 and U_6.

of the first three-times diffracted rays from the multiple Kirchhoff integral method.

The complex amplitude of a single diffraction on the antiblaze surface, Λ_1, divided by the incident complex amplitude, is

$$U_1 = K_1 \gamma_\alpha(\beta+\theta_i) \int_{\xi_0}^{\xi_1} \exp[ik\xi A][\cos(\beta+\theta_i) + \cos(\beta+\theta_r)]\psi(\theta_i)\psi(\theta_r)\,d\xi, \quad (8)$$

where

$$A \equiv \sin(\beta+\theta_i) + \sin(\beta+\theta_r). \quad (9)$$

To solve the shadowing problem and from the equivalent field principle which has been discussed in Eqs. (8) and (9),

if $\theta_i > \frac{\pi}{2} - \beta$, then let $\theta_i = \pi - 2\beta - \theta_i$ and $\psi(\theta_i) = -1$,

and if $\theta_r > \frac{\pi}{2} - \beta$, then let $\theta_r = \pi - 2\beta - \theta_r$ and $\psi(\theta_r) = -1$,

otherwise let $\psi(\theta_i) = 1$ and $\psi(\theta_r) = 1$;

if $\theta = \mathrm{Min}(\theta_i, \theta_r) \le \alpha - \frac{\pi}{2}$,

then let $\xi_0 = \eta_1 \sin(\alpha - \theta - \pi/2) / \sin(\beta + \theta + \pi/2)$,

otherwise let $\xi_0 = 0$.

Similarly, the complex amplitude of the ray which is incident on the antiblaze surface Λ_1 scattered to the blaze surface Λ_2 and then diffracted out is

$$U_3 = (ik^2 d K_1/4) \int_{\eta_0}^{\eta_1} \gamma_\alpha(\angle n_2, t)[I_A \cos(\alpha - \theta_r) + iI_B] \exp[ik\eta \sin(a - \theta_r)]\psi(\theta_i)\psi(\theta_r)\,d\eta, \quad (10)$$

where

$$I_A = \gamma_\alpha(\beta+\theta_i) \int_{\xi_0}^{\xi_1} [H_1(kt)\cos(n_1,t) + iH_0(kt) \times \cos(\beta+\theta_i)] \exp[ik\xi \sin(\beta+\theta_i)]\,d\xi, \quad (11)$$

$$I_B = \gamma_\alpha(\beta+\theta_i) \int_{\xi_0}^{\xi_1} [F(kt)\cos(n_1,t)\cos(n_2,t) + iH_1(kt)\cos(n_2,t)\cos(\beta+\theta_i)] \times \exp[ik\xi \sin(\beta+\theta_i)]\,d\xi, \quad (12)$$

and

$$F(x) \equiv \frac{1}{2}[H_2(x) - H_0(x)]. \quad (13)$$

In Eqs. (10)–(13),

if $\theta_i > \frac{\pi}{2} - \beta$, then let $\theta_i = \pi - 2\beta - \theta_i$ and $\psi(\theta_i) = -1$,

and if $\theta_r < \alpha - \frac{\pi}{2}$, then let $\theta_r = 2\alpha - \pi - \theta_r$ and $\psi(\theta_r) = -1$,

otherwise let $\psi(\theta_i) = 1$ and $\psi(\theta_r) = 1$;

if $\theta_i < \alpha - \frac{\pi}{2}$,

then let $\xi_0 = \eta_1 \sin(\alpha - \theta_i - \pi/2) / \sin(\beta + \theta_i + \pi/2)$,

and if $\theta_r > \frac{\pi}{2} - \beta$,

then let $\eta_0 = \xi_1 \sin(\beta + \theta_r - \pi/2) / \sin(\alpha + \pi/2 - \theta_r)$,

else let $\xi_0 = 0$ and $\eta_0 = 0$;

$$U_5 = (k^3 d K_1/16) \int_{\zeta_0}^{\zeta_1} \gamma_\alpha(\angle n_1, v)[I_C \cos(\beta+\theta_r) + iI_D] \exp[ik\xi \sin(\beta+\theta_r)]\psi(\theta_i)\psi(\theta_r)\,d\zeta, \quad (14)$$

where

$$I_C = \int_0^{\eta_1} \gamma_\alpha(\angle n_2, t)[I_A H_1(kv)\cos(n_2,v) + I_B H_0(kv)]\,d\eta, \quad (15)$$

and

$$I_D = \int_0^{\eta_1} \gamma_\alpha(\angle n_2, t)[I_A F(kv)\cos(n_2,v)\cos(n_1,v) + I_B H_1(kv)\cos(n_1,v)]\,d\eta, \quad (16)$$

In Eqs. (15) and (16) and in the interrelated Eqs. (11) and (12),

if $\theta_i > \frac{\pi}{2} - \beta$, then let $\theta_i = \pi - 2\beta - \theta_i$

and $\psi(\theta_i) = -1$,

and if $\theta_r > \frac{\pi}{2} - \beta$, then let $\theta_r = \pi - 2\beta - \theta_r$

and $\psi(\theta_r) = -1$,

otherwise let $\psi(\theta_i) = 1$ and $\psi(\theta_r) = 1$;

if $\theta_i < \alpha - \frac{\pi}{2}$,

then let $\xi_0 = \eta_1 \sin(\alpha - \theta_i - \pi/2) / \sin(\beta + \theta_i + \pi/2)$,

and if $\theta_r < \alpha - \frac{\pi}{2}$,

then let $\zeta_0 = \eta_1 \sin(\alpha - \theta_r - \pi/2) / \sin(\beta + \theta_r + \pi/2)$,

otherwise let $\xi_0 = 0$ and $\zeta_0 = 0$.

In Eqs. (8)–(16), $K_1 = (\cos(\beta + \theta_i))/(2d\cos\theta_i)$ and $\gamma_a(\theta)$ is the Fresnel amplitude reflectivity of the grating surface material when it is illuminated by the ray with a polarization and θ incident angle. $H_0(x)$, $H_1(x)$, $H_2(x)$ are the Hankel functions, defined as $H_n(x) = J_n(x) - jY_n(x)$, and t or v is the distance between two scattering points which are on the opposite facets of the same groove. From these formulae and the reciprocity, we get U_2, U_4, U_6 [9].

3. Calculation and discussion

With the equations given in Section 2.4, the stability and the self-consistency of the multiple Kirchhoff integral method are to be examined in Figs. 4–6.

Fig. 4 shows the stability of this method with calculation to the -1 order efficiency of a perfectly conducting blazed grating ($\alpha = 6°$ and $\gamma = 90°$), from the absolute value of U_2, U_4 and U_6 change by the number of intervals by which the grating facet is divided equally. The grating is mounted as a Littrow configuration. The incident and the diffracted angle are all 10°. The grating is incident by the P polarization plane electromagnetic wave (the direction of the electric vector is parallel to the rulings).

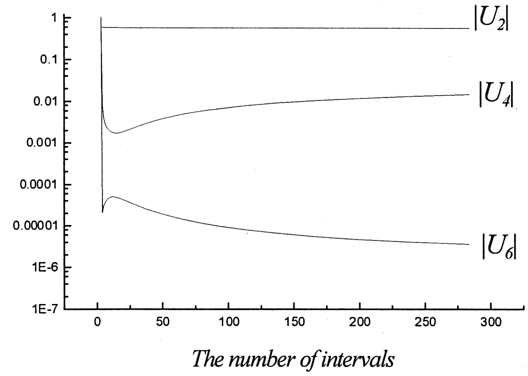

Fig. 4. The stability of multiple Kirchhoff integral algorithm. The absolute values of U_2, U_4, and U_6 change to the number of intervals in the course of every integral.

From the curves in Fig. 4, we may find that the (absolute) values of the complex amplitudes U_2, U_4 and U_6 converge if the number of intervals increases. Also, from these curves we can easily understand that U_6 goes to the stable point more slowly than U_4, and U_4 does so more slowly than U_2 only because of the effect of multiple integral. What our simulated calculation demonstrates is that the means of changing the number of intervals involves a great deal of time to get a sufficiently stable complex amplitude of U_5 and U_6. In addition, this method will produce increasingly higher accumulative errors when the number of intervals increases in an unrestrained manner because of the complexity of the method. Usually, the absolute ratio of U_6 to U_4 or U_4 to U_2 is much smaller than 1, so we can reduce the precision requirement of triple and/or double diffracted terms properly in the real course of calculating the efficiencies of diffracted orders. We can take advantage of the self-consistency of the method shown in Fig. 5 and Fig. 6 to analyze and estimate the calculations of the grating efficiency.

The self-consistency of one grating theory comes from the energy conversation law and means that the total efficiency of any perfectly conducting grating should be 1.

From our simulated calculations, we found that deciding how to choose the number of intervals in the course of once integral is the key problem which

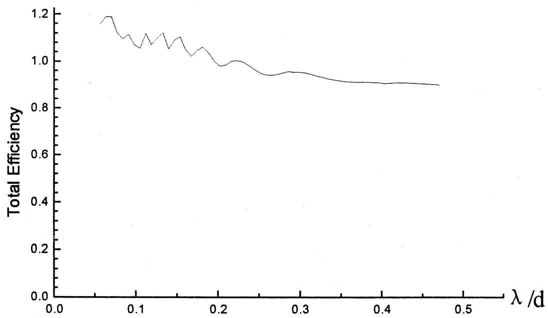

Fig. 5. The total efficiency curves of unpolarized light for a 4° blaze angle echelette grating and −1 Littrow mounting in the case of infinite conductivity.

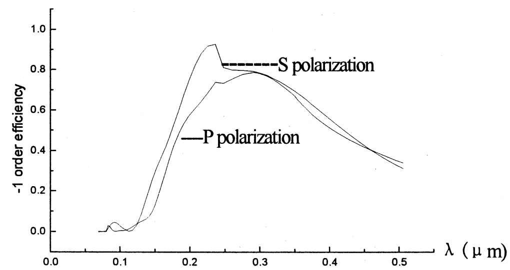

Fig. 7. The −1 order efficiency curves for a 16.74° blaze angle, 2400 groove/mm UV aluminum blazed grating, used in Littrow mount.

affects the precision and efficiency of the calculations. If we want to finish the whole calculation of any one order's efficiency curve or the total efficiency curve, we must deal with a very wide wavelength range. For example, under −1 order Littrow mounting conditions, the grating equation can be written as $\theta_i = \theta_r = \arcsin(\lambda/2d)$. Thus, from the optical sampling theorem (OST), we know that the length of one interval, in principle, should be less than $\lambda/10$ or $\lambda/5$, if what you care about is only the calculating precision. However, only from the OST, just with a present PC, we could not deal with the situation of $\lambda/2d \to 0$ only because the calculating quantity is too large (for instance, if we handle a grating with a 2° blazed angular, and when $\theta_i = \theta_r = 0.2°$, then the number of intervals on the blazed facet should be 1431, and the calculation of U_5 or U_6 is a triplex integral). However, when $\theta_i = \theta_r \to 90°$ or $\lambda/2d \to 1$, the number of intervals which is decided from OST and is equal to $\lambda/10$ turns out to be 5, and this situation cannot give any promise for the precision of the integral calculations.

Thus, in the following calculations, excluding the limit situation of $\lambda/d \to 0$, the number of intervals in once integral is taken to be fixed.

The total efficiency curves of perfectly conducting blazed gratings calculated with 40 intervals in each diffraction course are shown in Figs. 5 and 6.

In Fig. 5, the blazed angle of the grating is 4° and the grating is mounted with −1 order Littrow configuration. In Fig. 6, the blazed angle of the grating is 13° and the grating is mounted with −1 order fixed angular deviation. Both the grating in Fig. 5 and that in Fig. 6 are incident by unpolarized plane wave and both P and S polarization effects are taken into account together during the calculations. The total efficiency curves of the gratings shown in these figures depart from 1, because of the rounding-off error and accumulative error produced in the course of calculation, and because of the truncation error

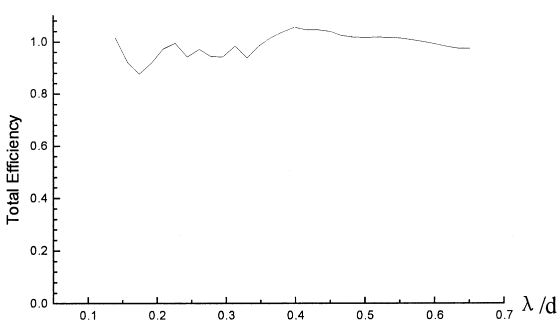

Fig. 6. The total efficiency curves of unpolarized light for a 13° blaze angle echelette grating, perfectly conducting, used with 45° between incident and −1 order diffracted beams.

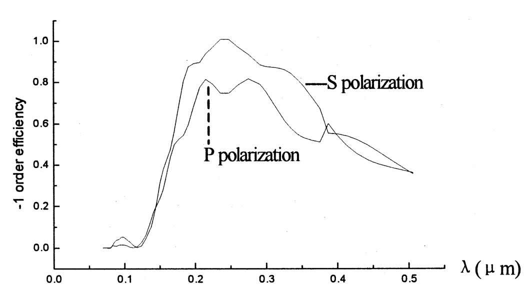

Fig. 8. The −1 order efficiency curves for a 8.28° blaze angle, 1200 grooves/mm UV aluminum blazed grating, used with 45° fixed angular deviation between incident and diffracted beams.

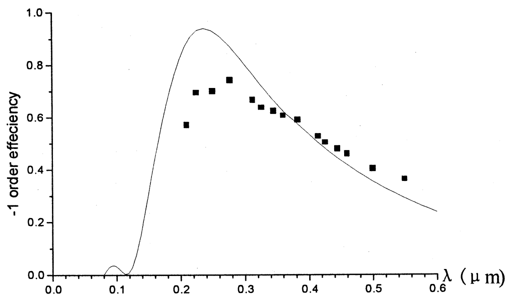

Fig. 9. The −1 order efficiency for a 0.24 μm blaze wavelength, 2400 grooves/mm UV aluminum blazed grating, used in near Littrow mount (10° between incident and −1 order diffract beam), while incident plane electromagnetic waves are unpolarized. The solid curve is from the calculation, and the dot is from the experiment.

produced from the neglecting of four-fold and more than four-fold diffractions (i.e. U_7, U_8 . . .).

However, from the calculations we have completed, we know that it is easy to control the total error of the total efficiency in the range of about 10% by choosing the number of the intervals to be in the range of 40–80 in the course of the calculation of once diffraction.

Since the self-consistency of the multiple integral method has been examined in Figs. 5 and 6, we can easily calculate the efficiencies of the real metal blazed gratings which work in the UV band where the optical index of the grating surface materials, which depend on the wavelength, must be taken into account [13]. For instance, the −1 order efficiency curves of aluminum blazed gratings of different parameters and which are used in different mounting model are given in Figs. 7 and 8.

In order to examine the reliability of the calculations of the multiple Kirchhoff integral method, in

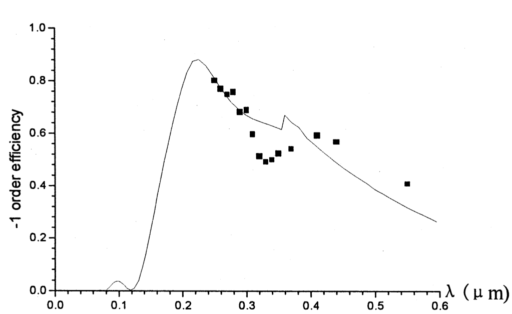

Fig. 10. As for Fig. 9 except blazed wavelength is 0.25 μm.

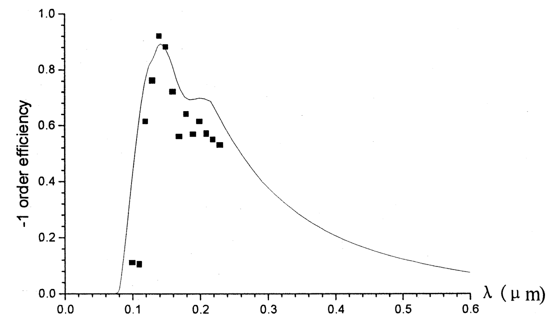

Fig. 11. As for Fig. 9 except blazed wavelength is 0.15 μm.

Figs. 9–12, the calculated −1 order's efficiencies of UV aluminum blazed gratings, while they are under near Littrow mounting conditions and the incident plane electromagnetic waves are unpolarized, are compared with the experimental result finished by Shuhong [12] in our laboratory two years ago.

From these comparisons of simulated calculations and the experimental results, we believe that the developed multiple Kirchhoff integral method is suitable for solving the efficiency problems and the anomalous behaviors of UV metal blazed gratings, since the calculated and the experimental data in Figs. 9–11 are almost coincident.

However, the experimental data in Fig. 12 do not show the anomalous behaviors which are found in the calculations. From analysis, we know that except for the calculating precision, the main reason of disagreement between the calculated and the experimental results is that the incident plane electromagnetic waves in the calculations are unpolarized. In contrast, the monochromatic incident waves in the experiment are obtained from the diffract grating

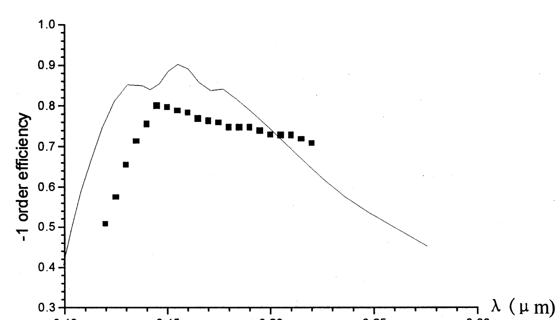

Fig. 12. As for Fig. 9 except blazed wavelength is 0.15 μm and groove number is 1200/mm.

inside the Seya-Namioka monochromator and are incompletely depolarized. Also, from Figs. 7 and 8, we know that the polarizations of the incident waves may have a great effect on the distribution of the efficiencies to the incident wavelengths.

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