Analytical calculation of diffraction order intensities for a hyperspectrometer

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Abstract. We employ a geometric optics approach to calculate the eikonal of a light field at the output of a diffraction grating in the immediate microrelief vicinity. Analytic relations to calculate the diffraction order intensities as functions of the grating step height, line spacing, wavelength of incident light, and incidence angle are deduced. By way of illustration, intensities of the diffraction orders for a blazed reflection grating with a 555-nm operating wavelength utilized in hyperspectrometers are calculated.

1. Introduction
Blazed reflective gratings have been actively employed in the devices for Earth remote sensing in the hyperspectral range [1 - 8]. In this case, gratings capable of generating the maximum intensity in a given diffraction order in a desired wave range are utilized. The numerical simulation of blazed diffraction gratings was discussed in sufficient detail in Ref. [9]. It is of interest to derive analytic relations to describe intensities of the diffraction orders of the grating. The analytic relations make it possible to speed up the process of designing and numerical investigation of a digital 'clone' (imitation model) of the hyperspectrometer.

2. Formulation of the problem
The aim of the work is to derive an analytic relation to describe intensities of the diffraction orders of a blazed diffraction grating as a function of its geometric parameters and an operating wavelength. For this purpose, one needs to solve the following problems:
- Using geometric optics approach, one needs to derive an analytic relation to describe the complex amplitude of a field at the diffraction grating output. The output of the diffraction grating is understood as a plane in the immediate vicinity of the grating microrelief.
- Deduce an analytic relation to describe amplitudes of the diffraction orders.
2.1. Geometric model of a grating step
For simplicity, the step of the diffraction grating is approximated by a tilted line \( t \). At the incidence angle \( \theta \), the light ray component lying in the plane of the grating profile (with a line spacing of \( d \)) passes through the point \( \xi \), with the reflected ray passing through the point \( \xi' \) at a height of \( h \) (Figure 1).

![Figure 1. Step profile for a diffraction grating approximated by a line.](image)

The complex amplitude of a diffraction order can be calculated using the relation [10]:

\[
U_m(\lambda) = \frac{1}{d} \int_0^d \exp(-2i\pi m\xi'/d)\exp(ik\phi(\xi'))d\xi',
\]

where \( \phi(\xi') \) is the eikonal of the reflected wave at the grating output, expressed as a function of \( \xi' \). The eikonal function takes the form:

\[
\phi(\xi') = \xi'\sin(\theta) - \xi'\sin(\theta) + l(\xi'),
\]

where \( \xi(\xi') \) is the point of ray incidence as a function of \( \xi' \) and \( l(\xi') \) is the optical path length between the input and output points.

We shall derive an explicit relation for the eikonal using a geometric optics model of the diffraction grating step (Fig. 1).

2.2. Relations to calculate the eikonal of a reflected wave at the diffraction grating output
From the model under study, we can easily derive important relationships for the angles:

\[
\alpha = \arctan(h/d) \\
\sigma = 90^\circ - \theta \\
\gamma = 2(\theta - \alpha) \\
\phi = 90^\circ + 2\alpha - \theta
\]

Assuming that the line \( t \) (Fig. 1) passes through the origin, we can write down the relation:

\[
y = x h/d
\]

Expressing the coordinates of the intersection of the lines \( BC \) and \( t \) via \( \xi' \), we obtain for \( BC \):

\[
h = \xi'\tan(\phi) + b \Rightarrow h = h - \xi'\tan(\phi) \Rightarrow y = x\tan(\phi) + h - \xi'\tan(\phi)
\]

Equating the relationships in Eqs. (4) and (5), we obtain:

\[
x \cdot h/d - x\tan(\phi) = h - \xi'\tan(\phi) \Rightarrow x = \frac{d(h - \xi'\tan(\phi))}{h - d\tan(\phi)}
\]

Substituting the relation for \( x \) from Eq. (6) into Eq. (4), we express the coordinates of the point \( C \) via \( \xi \):

\[
C \left( \frac{d(h - \xi'\tan(\phi))}{h - d\tan(\phi)}, \frac{b(h - \xi'\tan(\phi))}{h - d\tan(\phi)} \right)
\]
Using a similar reasoning, we can easily express the coordinates of the intersection point of the lines $AC$ and $t$ via $\xi$:

$$
\begin{aligned}
\begin{bmatrix}
\tan(\theta + \xi' - \theta) \\
\tan(\theta + \xi + \theta) \\
\tan(\theta + \xi' - \theta)
\end{bmatrix}
= \begin{bmatrix}
th(\theta + \xi' - \theta) \\
h(\theta + \xi + \theta) \\
h(\theta + \xi' - \theta)
\end{bmatrix}
\end{aligned}
$$

(8)

Based on Eqs. (7) and (8), we obtain:

$$
\xi = g_1(0, \varphi, h, d) \cdot \xi' + g_2(0, \varphi, h, d),
$$

(9)

where

$$
\begin{aligned}
g_1(0, \varphi, h, d) &= \frac{\tan(\theta)h(\theta + \xi + \theta)}{h(\theta + \xi' - \theta)\tan(\theta + \xi + \theta)}, \\
g_2(0, \varphi, h, d) &= \frac{hd(\theta + \xi' - \theta)}{h(\theta + \xi + \theta)\tan(\theta + \xi + \theta)}.
\end{aligned}
$$

(10)

Hereafter, the parameters of the functions $g_1$ and $g_2$ are dropped.

From a sine theorem, we can write down:

$$
AC = AB \sin(\varphi)/\sin(\gamma)
$$

(11)

$$
BC = AB \sin(\sigma)/\sin(\gamma)
$$

For the optical path length, we obtain:

$$
\ell(\xi') = [AC] + [BC] = |AB| \chi = (\xi' - \xi) \cdot \chi = \xi' \chi (1 - g_1) - \chi g_2,
$$

(12)

where

$$
\chi = (\sin(\varphi) + \sin(\sigma))/\sin(\gamma)
$$

(13)

Substituting (9) and (12) into (2), we get:

$$
\bar{\varphi}(\xi') = \xi' (1 - g_1)(\chi - \sin(\theta)) + g_2 (\sin(\theta) - \chi)
$$

(14)

After rearrangements, the eikonal is given by

$$
\bar{\varphi}(\xi') = (\chi - \sin(\theta)) + g_2 (\sin(\theta) - \chi)
$$

(15)

### 2.3. Relationships to calculate the complex amplitude of the diffraction order

The complex amplitude is calculated by substituting (15) into (10):

$$
U_m(\lambda) = \frac{1}{d} \int_0^d \exp(-2\pi i m \xi' / d) \exp(ik\bar{\varphi}(\xi')) d\xi' = 
$$

$$
= \frac{1}{d} \exp(ikg_2 (\sin(\theta) - \chi)) \int_0^d \exp\left(-2ik\xi' \left(\frac{\pi m}{kd} - \frac{1}{2}(1 - g_1)(\chi - \sin(\theta))\right)\right) d\xi'
$$

(16)

Taking the integral in Eq. (16) and doing further rearrangements we find an expression for $U_m$:

$$
U_m(\lambda) = \exp(ia) \exp(-ib) \text{Sinc}(b),
$$

(17)

where

$$
\begin{aligned}
a &= k \left(\sin(\theta) - \chi\right) g_2, \\
b &= kd \left(\frac{\pi m}{kd} - \frac{1}{2}(1 - g_1)(\chi - \sin(\theta))\right)
\end{aligned}
$$

(18)

Thus, we have derived a simple analytic relationship in Eq. (17) that enables the amplitude of a diffraction order to be calculated as a function of the grating parameters (line spacing and step height), the angle of incidence on the grating step, and the incident wavelength.

This approach is also suitable for gratings with a more complex profile, e.g. that defined by second-order curves. The major condition to be met is the possibility of deriving an analytic expression for the intersection point and an incident ray. This condition is met for the second-order curves. It is worth noting that the approximation of more complex profiles by a linear profile for gratings utilized in hyperspectrometers is sufficiently accurate, with the use of more intricate formulae not leading to considerable deviations of the diffraction order intensity values from the approximate estimates.
3. Calculation of the diffraction order intensity

The intensity of the diffraction orders can be calculated using a standard relationship:

$$I_m(\lambda) = |U_m(\lambda)|^2 \frac{\cos(\theta_m)}{\cos(\theta)}$$

where $\theta_m$ is the reflection angle of a ray component depending on the diffraction order $m$ in the grating profile plane of interest.

For the computer-aided simulation of the performance of a digital 'clone' of hyperspectrometer, while aiming to speed up the computation, we utilize an average value of the coefficient calculated using the formula:

$$C_m(\lambda) = \eta^{-1} \sum_{i=1}^{\eta} C_m^i(\lambda)$$

where $\eta$ is the number of incident rays that hit the device registration plane.

Making use of the above-derived relationships, we can plot curves for the diffraction order intensities versus the incident wavelength. To these ends, we choose a grating that produces the maximum intensity in the first diffraction order at a wavelength of $\lambda = 555 \text{nm}$. Figures 2 and 3 present simulation results for several positive and negative diffraction orders.

![Figure 2](image1)

**Figure 2.** Intensity profiles of the negative diffraction orders for a blazed diffraction grating at a wavelength of $\lambda = 555 \text{nm}$ (at $\theta = 0$).

![Figure 3](image2)

**Figure 3.** Intensity profiles for the positive diffraction orders of a blazed diffraction grating at a wavelength of $\lambda = 555 \text{nm}$ (at $\theta = 0$).
From Figs. 2 and 3, the blazed grating is seen to direct the maximum intensity of light energy to the negative diffraction orders.

For the grating to direct the maximum intensity to a positive diffraction order, the light ray needs to travel in the opposite direction through the point $\xi'$ (Fig. 1). Using a similar reasoning, it is possible to derive a relationship for the eikonal at the grating output, $\bar{\varphi} = \bar{\varphi}(\xi)$ and calculate the integral in Eq. (1) or, alternatively, just use the following replacements in the already derived relations:

$$g_1(\theta,\varphi,h,d) \rightarrow G_1(\theta,\varphi,h,d)$$

$$g_2(\theta,\varphi,h,d) \rightarrow G_2(\theta,\varphi,h,d)$$

where

$$G_1 = 1/g_1$$

$$G_2 = -g_2/g_1$$

As the result of the replacements in Eqs. (21) and (22), the curves in Fig. 2 will describe the positive diffraction order, with Fig. 3 describing the negative diffraction order.

4. Conclusion

We have employed a geometric optics approach to describe the eikonal function of a light wave and derived an analytic relationship for calculating the intensity of diffraction orders as a function of grating parameters and the incidence angle of a light wave. By way of illustration, we discussed the calculation of intensity coefficients for a blazed diffraction grating operating at a 555-nm wavelength.

The simulation results agree well with Ref. [9] and can be utilized for the design of hyperspectral devices. The approach proposed is also suitable when designing diffraction gratings with a more complex profile, e.g. that described by second-order curves. In the future, we plan to compare the calculated data with the results obtained in the optical experiment. To do this, we are going to make an appropriate diffraction grating using the technologies available in our Institute [11-20], and then study its operation on an optical stand [20-25].

5. References

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