Scalar theory of transmission relief gratings

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A simple formula is derived that allows evaluation by a single integration the diffraction efficiencies of transmission relief gratings when they support a great number of orders. Validity of the method is demonstrated by comparison with a rigorous differential method.

1. Introduction

Scalar theory of gratings has attracted the attention of scientists for quite some time [1–6]. Its application offered one of the rare possibilities to deal satisfactory with light diffraction by simple formulations before rigorous electromagnetic theories were developed. After a massive attack by numerical methods [7] scalar theories almost went in obliviation, although Maystre commented on their importance: *However is must be emphasized that such a theory is very valuable when λ/d is low* [8]. when the λ/d ratio is small, which is typical because transmission gratings tend to have coarse spacing and shallow modulation, it is an unnecessary luxury to use rigorous theories. Because of the large number of propagating orders they require excessive and wasteful amounts of computer time. It might be noted that the importance of scalar theories is indicated by the fact that the most recent reference in this field is given by the authors who have contributed the most to the development of rigorous methods [6].

Since publication of ref. [6] the role of surface relief gratings has greatly increased. Undoubtly the most popular use, by far, is their application in CD players [9] and in similar systems for optical data storage [10]: symmetrical groove profile transmission gratings are used to split laser beams into three parts, the zeroth order being used for signal recovery and the $\pm$1st orders providing the track centering signal. Not so obvious are the many possibilities for beam splitting in numerous research projects.

The aim of this paper is to present a simple approach for deriving a closed formula capable of evaluating the diffraction efficiencies of surface relief transmission gratings by a single integration, provided only that $\lambda/d \ll 1$. Section 3 contains numerical examples that demonstrate the possibilities and restrictions of the method and the comparison with the results of rigorous differential method is emphasized. An unexpected result was that the simpler approach gave better results than the more sophisticated one of section 3.4.

2. Theoretical considerations

A plane monochromatic wave is incident at an angle θ_0 on a relief grating whose profile is defined by $y=f(x)$. The y-axis is perpendicular to the grating plane and the x-axis is perpendicular to the grooves. The grating surface separates two semi-infinite media with refractive indices n_1 and n_2.

The *main assumption* is that $f(x)$ varies slowly

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with respect to wavelength: the reflected and transmitted fields, E_R and E_T respectively, are assumed equal to the corresponding fields that exists when light is incident upon a plane interface, i.e.

$$E_T(x,y)|_{y=f(x)} = T\exp\{i[\alpha_0 x - \chi_{1,0} f(x)]\}, \quad (1)$$

$$\alpha_0 = kn_1 \sin\theta_0, \quad \chi_{1,0} = kn_1\cos\theta_0, \quad k = 2\pi/\lambda, \quad (2)$$

and T is the transmission coefficient that is derived assuming normal incidence:

$$T = 2n_1/(n_1+n_2). \quad (3)$$

In deriving eq. (1) we have taken into account that incident wave field value calculated in a point (x, $y=f(x)$) on the profile is equal to

$$E_i = \exp\{i[\alpha_0 x - \chi_{1,0} f(x)]\}. \quad (4)$$

It is well known that below the modulated region $y < \min f(x)$ the transmitted field can be represented in the form of the Rayleigh expansion:

$$E_T(x,y) = \sum_m T_m \exp[i(\alpha_m x - \chi_{2,m} y)], \quad (5)$$

with

$$\alpha_m = \alpha_0 + mK, \quad K = 2\pi/d, \quad (6)$$

$$\chi_{2,m} = (k^2 n_2^2 - \alpha_m^2)^{1/2}, \quad (7)$$

and $\{T_m\}$ are diffraction orders amplitudes.

A *second assumption* is the so-called *Rayleigh hypothesis*, i.e. that representation (5) is valid not only outside the modulated region, but all over the entire lower medium. The validity of this hypothesis has been widely discussed during the last decade [8], so that its theoretical and numerical restrictions are well known. For the shallow and slowly varying profiles under consideration here it works quite well, as shown in the next section.

Uniqueness of the field in the second medium leads to the following equation on the grating profile:

$$\sum_m T_m \exp\{i[\alpha_m x - \chi_{2,m} f(x)]\} = T\exp\{i[\alpha_0 x - \chi_{1,0} f(x)]\}, \quad (8)$$

that enables us to obtain a closed form expression for diffraction orders amplitudes. Multiplying eq. (8) with

$$(1/d)\exp\{-i[\alpha_m x - \chi_{2,m} f(x)]\}$$

and integrating over one period one obtains that

$$T_m = \frac{T}{d}\int_0^d \exp[-imKx - i(\chi_{1,0} - \chi_{2,m}) f(x)]\,dx. \quad (9)$$

In evaluating eq. (9) it is assumed that

$$\frac{1}{d}\int_0^d \exp[-i(n-m)Kx - i(\chi_{2,m} - \chi_{2,n}) f(x)]dx = \delta_{mn}, \quad (10)$$

where δ_{mn} is the Kroneker's symbol. Eq. (10) is valid in the limit $h \to 0$, but also when $\lambda/d \to 0$. In the last case $\chi_{2,m} \to \chi_{2,n} \to kn_2\cos\theta_{2,0}$, i.e. all diffraction orders are gathered around the zeroth transmitted wave. Strictly speaking, eq. (10) assumes that all orders carrying significant amount of energy should have negligible angular deviation from the specular transmitted wave.

In a similar manner reflected orders amplitudes B_m can be represented in closed form:

$$B_m = \frac{R}{d}\int_0^d \exp[-imKx - i(\chi_{1,0} + \chi_{1,m}) f(x)]\,dx, \quad (11)$$

where

$$R = (n_1 - n_2)/(n_1 + n_2). \quad (12)$$

Eq. (11) coincides with the formula derived by Beckmann [5] at normal incidence, when the substrate is not perfectly conducting.

3. Discussion

In the case of well known simple profiles eqs. (9) and (11) can be evaluated with a pocket calculator:

3.1. *Sinusoidal gratings*

When grating profile is described by a sine function $f(x) = \frac{1}{2}h\sin(Kx)$ the mth order amplitude is expressed by the mth order Bessel function

$$T_m = \frac{2n_1}{n_1+n_2} J_m[\tfrac{1}{2}h(\chi_{1,0} - \chi_{2,m})], \quad (13)$$

describing the well known case of Raman-Nath diffraction [11,12].

3.2. Lamellar gratings

The validity of eq. (9) is demonstrated for lamellar gratings in figs. 1 and 2. Good coincidence is obtained with results from a rigorous differential formalism [13], even with relatively moderate angles of incidence, despite the fact that the representation (3) is for normal incidence. Significant discrepancy is observed only at high angles of incidence, where angular deviation between zeroth and higher diffraction orders becomes greater. Of course scalar theory can not predict any threshold anomalies as higher order cut-off is not included.

It could be useful to use eq. (9) to predict groove depth values for which grating exhibits some specific properties. For example, zero efficiency in the zeroth transmitted order at normal incidence is given by the following equation

$$\frac{c}{d}\exp[-\mathrm{i}(n_1-n_2)kh]+\frac{d-c}{d}=0\,, \tag{14}$$

where c/d is the so called filling ratio of the profile.

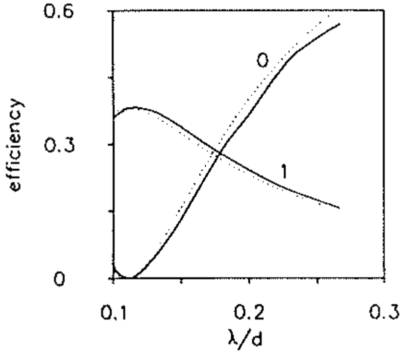

Fig. 1. Spectral dependence of diffraction efficiency in the zeroth and −1st transmitted orders at normal incidence of lamellar grating with filling ratio 0.5. Period $d=3$ µm, groove depth $h=0.3$ µm. Solid lines – rigorous differential formalism, dotted lines – eqs. (3) and (9). $n_1=1.55$, $n_2=1$.

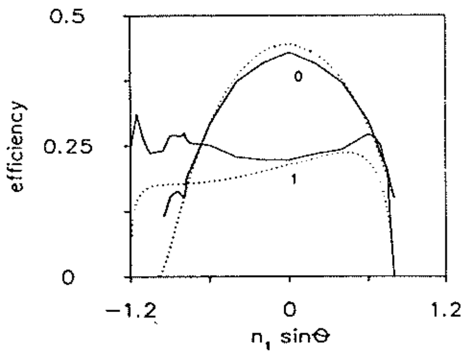

Fig. 2. Angular dependence of diffraction efficiency in the zeroth and −1st transmitted orders of lamellar grating with filling ratio 0.5. Period $d=3$ µm, groove depth $h=0.3$ µm, wavelength $\lambda=0.6$ µm. Solid lines – rigorous differential formalism, dotted lines – eqs. (3) and (9). $n_1=1.55$, $n_2=1$.

3.3. Blazed gratings

Results for diffraction efficiency in different transmission orders are shown in fig. 3 for a wide spectral region. Two blaze angles are treated (10° and 15°).

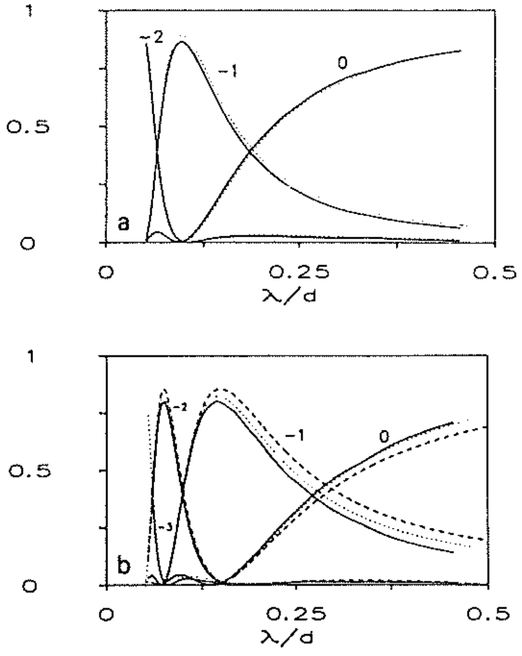

Fig. 3. Spectral dependence of transmitted orders diffraction efficiency of echelette diffraction grating with blaze angle 10° (a) and 15° (b). Period $d=3.33333$ µm, apex angle 90°. Solid lines – rigorous differential formalism, dotted lines – eqs. (3) and (9), dashed line – eqs. (9) and (19). $n_1=1.55$, $n_2=1$.

Good coincidence is observed between results of rigorous and scalar theories, even when the λ/d ratio is relatively large. Surprising is that even for large angles of incidence eqs. (3) and (9) can still produce good results (fig. 4, with blaze angle 18°).

It will be noticed that despite the assumption of lossless materials for transmission gratings the peak first order efficiency always lies in the 80 to 85% range, even when there is very little energy in the zeroth and second orders. The explanation lies in the fact that such gratings will always diffract a certain amount backward, towards the incident – the resin-air interface acts like a low efficiency reflection grating.

It must be pointed out that the blaze wavelength could easily be determined from eq. (9), by assuming that the main contribution to the diffraction process is given by the long facet, whose geometry is defined by the equation:

$$f(x)=x\tan\varphi_B\,, \qquad (15)$$

where φ_B is the groove angle. Maximum efficiency in the mth order is obtained when

$$m\frac{2\pi}{d}=-(n_1\cos\theta_{1,0}-n_2\cos\theta_{2,m})\frac{2\pi}{\lambda}\tan\varphi_B\,. \qquad (16)$$

After some simple transformations eq. (16) could be expressed as

$$n_2\sin\psi_2=n_1\sin\psi_1\,, \qquad (17)$$

where

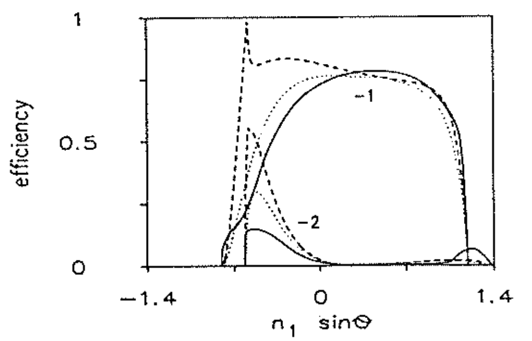

Fig. 4. Angular dependence of diffraction efficiencies in −1st and −2nd transmitted orders of echelette grating with blaze angle of 18°. Wavelength $\lambda=0.6328$ μm. The other parameters are as stated in fig. 3.

$$\psi_2=\varphi_B-\theta_{2,m}\,,\quad \psi_1=\varphi_B-\theta_{1,m}\,. \qquad (18)$$

Eq. (17) is nothing but the Snell's law, i.e. the mth order efficiency exhibits a maximum when its direction of propagation corresponds to the direction of light refracted from the large facet.

3.4. Is higher precision more precise?

We do not argue with the general statement that higher precision is more precise, but the problem investigated here exhibits a curious property in presenting an example how an a priori true statement may not always be correct. Indeed, it appears to be much more correct to replace assumption (3) with the following hypothesis: the transmitted field is equal to the field refracted by a plane that is locally tangential to the profile, i.e. the transmission coefficient is presented in the form:

$$\tilde{T}(x)=\frac{2\tilde{\chi}_1}{\tilde{\chi}_1(x)+\tilde{\chi}_2(x)}\,, \qquad (19)$$

where $\tilde{\chi}_1$ and $\tilde{\chi}_2$ are the incident and refracted wavevector components along the $\tilde{y}$ axis (fig. 5) that is locally normal to the profile. We have made calculations using this assumption (19) instead of (3) and its result are much less precise, see figs. 3b and 4, where assumption (19) produces false blazing for high angles of incidence. This paradox can be easily understood from the following speculations:

In the case of blazed gratings we are interested in the contribution of the long facet. Intuitively, when the angle between incident wavevector and direction

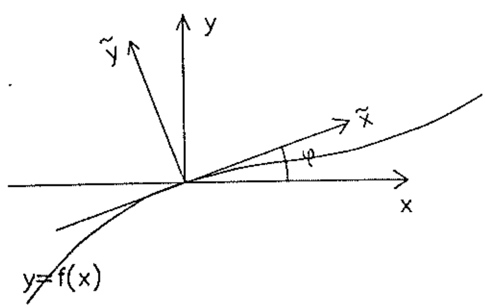

Fig. 5. Schematical representation of grating profile $y=f(x)$ with two coordinate systems: general Oxy and local O$\tilde{x}\tilde{y}$ ones.

normal to this facet increases, one expects that the transmittance decreases (in TE polarization), i.e. total efficiency in transmitted orders has to go down. On the other hand, the coefficient represented by eq. (19) is *growing* instead of decreasing. In fact, when light is refracted by a plane surface, the decreasing of transmitivitty is due to the factor of $\tilde{\chi}_2/\tilde{\chi}_1$ in the efficiency representation:

$$\eta_T = |\tilde{T}|^2 \tilde{\chi}_2/\tilde{\chi}_1 , \qquad (20)$$

while the corresponding diffraction efficiency in the mth order is given by the modulus square of the amplitude multiplied by the factor of

$$\chi_{2,m}/\chi_{1,0} . \qquad (21)$$

For negative angles of incidence and for orders of negative number, in the case when they are propagating close to the negative direction of y-axis factor (21) when multiplied with (19) could result in much higher efficiency values than the real ones. Thus the false blazing in fig. 4 appears if eq. (19) is used instead of eq. (3).

Acknowledgement

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References

[1] R.D. Hatcher and J.H. Rohrbaugh, J. Opt. Soc. Am. 46 (1956) 104.
[2] J.H. Rorhbaugh and R.D. Hatcher, J. Opt. Soc. Am. 48 (1958) 704.
[3] R.P. Madden and J. Strong, Some concepts of classical optics (Freeman, San Francisco, 1958) p. 605.
[4] P. Beckmann and A. Spizzichino, The scattering of electromagnetic waves from rough surfaces (Pergamon, Macmillian, London, New York, 1963).
[5] P. Beckmann, in: Progress in optics, Vol. VI, ed. E. Wolf (North-Holland, Amsterdam, 1967) p.53
[6] E.G. Loewen, M. Neviere and D. Maystre, J. Opt. Soc. Am. 68 (1978) 496.
[7] See for example: Electromagnetic theory of gratings, ed. R. Petit (Springer, Berlin, Heidelberg, New York, 1980).
[8] D. Maystre, in: Progress in optics, ed. E. Wolf, Vol. XXI (Elsevier Sciece, 1984) p. 19.
[9] G. Bouwhuis and J.J.M. Braat, Appl. Optics 17 (1978) 1993.
[10] T. Musha, K. Kata and Kitto, Method for reproducing optical information on a record medium along tracks, U.S. Patent 4425636.
[11] C.V. Raman and N.S.N. Naht, Proc. Ind. Acad. Sci 2A (1935) 413.
[12] E.G.H. Lean, in: Introduction to integrated optics, ed. M.K. Barnoski (Plenum, New York and London, 1974), ch. XIV.
[13] M. Neviere, P. Vincent and R. Pepit, Nouv. Rev. Opt. 5 (1974) 1.