Bragg properties of efficient surface relief gratings in the resonance domain

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Abstract

Closed form analytical solutions of diffraction efficiency for transmission surface relief gratings in the resonance domain are presented. These are obtained by modeling the surface relief gratings with equivalent graded index gratings having Bragg properties, so as to allow for an optimum choice of grating parameters that would lead to high diffraction efficiencies. The calculated and experimental results reveal that the diffraction efficiency can be greater than 85% with optimized grating parameters within their certain strict limits.

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Surface relief gratings in the resonance domain, where the grating period is comparable to that of the illumination wavelength, have a unique diffraction efficiency peak [1,2]. The physical nature of this peak is not yet understood completely [3,4]. In order to analyze such gratings, it is usually necessary to resort to extensive numerical methods of rigorous diffraction theory, presented for example in [1,2,5–8]. This is particularly so when optimizing the various grating parameters and trade-offs for surface relief gratings in the resonance domain in order to obtain the best diffraction efficiencies.

In this paper, we present a new approach for analyzing resonance domain surface relief gratings. It is based on “equivalent” sinusoidal graded index gratings model, and provides analytic, closed form solution for evaluating the performance of surface relief gratings with arbitrary groove shapes and diffraction efficiencies. Moreover, the model explains the unique diffraction efficiency peak and provides constraints on the grating parameters for which high diffraction efficiencies can be achieved.

We begin by considering a basic surface relief grating, recorded on a planar substrate, that is illuminated with a monochromatic oblique plane
wave of wavelength \( \lambda \) at an incidence angular orientation of \( \theta_{\text{inc}} \). The period of this grating is \( \Lambda_z \), and the grooves are slanted for obtaining high diffraction efficiency. The relevant parameters and geometry of one groove from such a grating are depicted on the Fig. 1. The refractive index of groove material is \( n_M \), refractive index of upper layer \( n_i \), maximum depth of grooves \( h_{\text{max}} \) measured normal to the plane substrate. The distribution of the refractive index \( n \) of the groove has the values of either \( n_i \) or \( n_M \). Finally the normalized groove shape is defined by function \( g(\chi) \), where the normalized coordinate \( \chi \) ranges from 0 to 1, within a single grating groove, and \( 0 \leq g(\chi) \leq 1 \).

In dealing with slanted grooves, we found it convenient to rotate the coordinate system by a slant angle \( \phi_0 \), whose value must be optimized. In the rotated coordinate system the grooves are characterized by a normalized coordinate \( \chi_z \), a normalized “slanted groove shape” \( g_z(\chi_z) \), a slanted grating period \( \Lambda_z = \Lambda \cos \phi_0 \) and a slanted maximum depth of groove \( h_{\text{max},z} = h_{\text{max}} / \cos \phi_0 \). Applying usual coordinate rotation equations, followed by simple algebraic manipulations, yields

\[
g_z(\chi_z) = g(\chi) \quad \text{and} \quad \chi_z = \chi - pg(\chi) \tag{1}
\]

where \( p \) is the “slant parameter” defined as \( p = h_{\text{max}} \tan \phi_0 / \Lambda_z \).

We now develop the sinusoidal graded index model of the surface relief grating with slanted grooves. We begin by approximating \( n^2 \) with a two-dimensional complex Fourier series, as

\[
n^2 = n_0^2 + \Delta n_M^2 \sum_j G_j \exp(i2\pi j\chi_z), \tag{2}
\]

where \( \Delta n_M^2 = n_M^2 - n_i^2 \), and a slant angle \( \phi_0 \), which is incorporated in \( \chi_z \) (see Eq. (1)), must be optimized. The essentially constant parameters \( n_0 \) and \( G_j \) can be determined by routine mathematical least square approximation, to yield

\[
n_0^2 = \langle n^2 \rangle, \quad G_j = \langle n^2 - n_0^2 \exp(-i2\pi j\chi_z) \rangle \tag{3}
\]

where \( \langle \cdot \rangle \) denotes averaging within a single grating groove, both in width and height. The mean-square refractive index \( n_0^2 \) in Eq. (3) is calculated by integration of function \( n_0^2 \) along the normal to the grating, to yield

\[
n_0^2 = n_i^2 + \Delta n_M^2 \bar{g}, \quad \text{with} \quad \bar{g} = \int_0^1 g(\chi) \, d\chi. \tag{4}
\]

The value of the dominant first harmonic term coefficient \( G_1 \) is found by integration of piecewise constant function \( n^2 \) along the slant angle \( \phi_0 \) direction, to yield

\[
G_1 = \int_0^1 g_z(\chi_z) \exp(-i2\pi \chi_z) \, d\chi_z. \tag{5}
\]

We now introduce a refractive index modulation term \( \Delta n \), which is derived by comparing Eq. (2) to that obtained for sinusoidal graded index gratings [9], as

\[
\Delta n = \frac{\Delta n_M^2}{n_0} |G_1|. \tag{6}
\]

The refractive index modulation \( \Delta n \) in Eq. (6) depends on the difference between \( n_M \) and \( n_i \), the groove profile shape and slant parameter \( p \). In order to determine the “equivalent” graded index grating, which best characterizes the surface relief grating, it is necessary to properly choose the slant angle \( \phi_0 \) or alternatively the slant parameter \( p \). Denoting \( p \), as that value of \( p \) at which the maxi-
Eq. (7) leads to the dominant “equivalent” graded index grating that corresponds to a specific surface relief grating. Such an equivalent grating thus simulates most accurately the surface relief grating in terms of the highest possible value of Δn, i.e. Δn = Δn₁. Specifically Eqs. (4) and (5) together with Eqs. (1) and (7) essentially denote the most important relations between the surface relief grating and its sinusoidal graded index grating model. Together they simplify the complicated calculation of diffraction efficiencies for surface relief gratings in the resonance domain to those of relatively simple calculation for sinusoidal graded index model gratings.

Besides the dominant equivalent graded index grating with pᵣ and φᵣ, there are additional gratings with p and φ₀ that degrade the overall efficiency. In general, it is necessary to consider only those additional gratings, which have relatively high Δn. In particular, only those with |Δn/Δn₁| ≥ δₗow, where δₗow is a fixed small threshold value. In other words, we consider only additional gratings with p between boundaries pₗow and pₗow defined by equations pₗow = pᵣ ± Δpₗow and |Δn/Δn₁|p=pₗow = δₗow.

As a representative example we investigate the surface relief grating of slanted sinusoidal groove shape characterized by a relative groove peak position qᵣ, with 0 ≤ qᵣ ≤ 1 within the groove. In accordance to Eqs. (4) and (5), g = 0.5, pᵣ = qᵣ − 0.5 and the parameters G₁ and n₀ are

$$|G₁| = \frac{1}{2} \left| J₁(\pi(p-pᵣ)) / \pi(p-pᵣ) \right|, \quad n₀ = \sqrt{(n_M^2 + n_i^2)/2}. \tag{8}$$

Eq. (8) indicates that G₁, and consequently Δn of Eq. (6), have maximum values G₁ = 0.25 and Δn₁ = 0.25Δn_M²/n₀ at p = pᵣ, and side lobes. In this example, Δpₗow = 1.052, in accordance with a threshold value δₗow which was chosen as the ratio of the first side lobe peak to the maximum value.

For an arbitrary slant parameter p, the jth order Bragg conditions [9] can be written as

$$s_j^2 + c_j^2 = 1, \tag{9}$$

where, in our notations, s_j and c_j are

$$s_j = \frac{n₁}{n₀} \sin \theta_{inc} - j \frac{λ}{n₀A_x}, \quad c_j = \sqrt{1 - s_j^2 - j \frac{λ}{n₀A_x} p}. \tag{10}$$

Solving Eqs. (9) and (10) leads to the Bragg incidence angles θ_{inc,j} at wavelength λ for the resonance domain surface relief grating, as

$$n₁ \sin \theta_{inc,j} = \frac{J_j λ}{2A_x} - \frac{A_j p}{h_{max}} \left[ \frac{n₀^2}{1 + (A_j p/h_{max})^2} \right]^{1/2}. \tag{11}$$

The dominant +1st Bragg incidence angle θ_{inc,1} of the surface relief grating can be obtained from Eq. (11) with j = +1 and p = pᵣ.

Using the equivalent grating model, the calculation of the +1st order diffraction efficiency η₁ for highly efficient surface relief gratings, is now reduced to exploiting the relatively simple closed form analytic relation from the theory of the sinusoidal graded index grating [9], of

$$η₁ = \sin^2 \left( \sqrt{v_1^2 + ξ₁^2} \right) \left[ 1 + (ξ₁/v₁)² \right]^{-1}. \tag{12}$$

The parameters v₁ and ξ₁ are now specific for surface relief gratings, where ξ₁ for either TE or TM polarization is

$$ξ₁ = \frac{πh_{max}n₀}{2c₁λ} \left[ 1 - s_i^2 - c_i^2 \right], \tag{13}$$

and v₁ is different for TE and TM polarizations, as

$$v_{1TE} = \frac{πh_{max}}{2c₁λ} \frac{(n_M^2 - n_i^2)}{n₀} G₁s, \tag{14}$$

and

$$v_{1TM} = v_{1TE} \left\{ 1 - \frac{1}{2} \left( \frac{λ}{n₀A_x} \right)^2 \left[ 1 + \left( \frac{λpᵣ}{h_{max}} \right)^2 \right] \right\} \tag{15}$$

with c₀, c₁, s₁ defined by Eq. (10) when p = pᵣ.

Using Eqs. (5) and (12)–(15), we can draw several important conclusions. Letting ξ₁ = 0 in...
Eq. (12), is equivalent to satisfying the Bragg condition whereby $\eta_1$ becomes the Bragg efficiency $\eta_{\text{Bragg}}$. Then for a specific value of $\eta_{\text{Bragg}}$, the depth of groove $h_{\text{max}}$ can be found as a function of grating period $\Lambda$. Another interesting conclusion derived from Eqs. (5) and (12)–(15) is that in our treatment the Bragg efficiency of surface relief transmission gratings in the resonance domain is fully determined by the first Fourier coefficient of normalized slanted groove shapes calculated in the dominant slant direction of equivalent graded index grating. Still another conclusion is that surface relief gratings with different groove shapes will have the same Bragg efficiency when the Fourier coefficients of the normalized slanted groove shapes are equal. This conclusion is in agreement with the empirical criterion of “equivalence rule” for surface relief gratings [1,10].

Any small deviation of the incidence angle $\theta_{\text{inc}}$ from the Bragg incidence angle $\theta_{\text{inc}}^{\text{up}}|_{p=p_{\text{low}}}$ or deviation of the illumination wavelength from the Bragg wavelength at given Bragg angle, corresponds to varying the parameter $\zeta_1$, i.e. $\zeta_1 \neq 0$. This leads to a small relative reduction of the Bragg efficiency to $\eta_{\text{mis}}\eta_{\text{Bragg}}$, where the reduction factor is $\eta_{\text{mis}} (0.8 \lesssim \eta_{\text{mis}} \leq 1)$. From Eq. (12) we can readily determine analytical expression for the angular $\Delta\theta_{\text{inc,low}}$ and spectral $\Delta\lambda_1$ selectivities for highly efficient surface relief gratings as the bandwidth of diffraction efficiency response corresponding to the threshold level $\eta_{\text{mis}}\eta_{\text{Bragg}}$.

In order to determine the constraints of our approach, we must include in the analysis the degrading influence of additional gratings with slant parameter $p$ between boundaries $p_{\text{low}}$ and $p_{\text{up}}$. In accordance to Eq. (11), when $j = -1$, some of the light from each additional graded index grating, in particular for increasing values of $\Lambda_x/\lambda$, will be diffracted into the $-1$st order instead of the $+1$st order. To ensure that this undesirable diffracted light is minimal, the Bragg incidence angle $\theta_{\text{inc,low}} = \theta_{\text{inc,-1}}|_{p=p_{\text{low}}}$ of the “worst case” additional grating with $p = p_{\text{low}}$ must be sufficiently different from the $+1$st Bragg incidence angle $\theta_{\text{inc,1}}|_{p=p_0}$ of the dominant equivalent grating. In such a case the diffraction efficiency $\eta_1$ at the boundary $\theta_{\text{inc,low}}$ should be lower than $\eta_{\text{mis}}\eta_{\text{Bragg}}$ and, in the worst case, becomes

$$\eta_1 \bigg|_{\theta_{\text{inc,-1}}} = \eta_{\text{mis}}\eta_{\text{Bragg}}.$$  

Eq. (16) gives main restriction of applicability of our model. For a given groove depth $h_{\text{max}}$, the ratio $\Lambda_x/\lambda$ is constrained to be smaller than an upper bound value $\Lambda_x/\lambda$. This upper bound value is found by substituting Eq. (12) with $j = +1$ and $p = p_0$ and also Eq. (11) with $j = -1$ and $p = p_{\text{low}}$ into Eq. (16).

To verify our model, we performed numerical calculations using rigorous coupled wave analysis [1,5,6]. We found that the results with our analytic model are in agreement with the numerical calculations, especially those for deep gratings [11] as depicted by thin and thick curves in Fig. 2. For example, for symmetrical sinusoidal gratings with $\lambda/\Lambda_x = 1.414$, $h_{\text{max}}/\Lambda_x = 1.9$ and $n_M = 1.66$, the agreement for diffraction efficiency values is within 3% over the incidence angles ranging from 34° to 54°, with the Bragg incidence angle of 45°. This is shown in Fig. 3.

![Fig. 2. The diffraction efficiency of the +1st order as a function of groove depth to period ratio $h_{\text{max}}/\Lambda_x$ for symmetrical sinusoidal surface relief gratings. The Bragg incidence angle was 45°, ratio of readout illumination wavelength to the period $\lambda/\Lambda_x = 1.414$, refractive index of grooves $n_M = 1.50$, 1.66 and 2.0, and TE polarization. The thick-line curves are analytically calculated within the equivalent grating model of this paper, whereas the thin-line curves are numerically calculated by the rigorous coupled wave theory [11]. Analytical: - - - $n_M = 1.50$, $n_M = 1.66$, $n_M = 2.0$. Numerical: - - - $n_M = 1.50$, $n_M = 1.66$, $n_M = 2.0$.](image-url)
To determine the relationship between the depth of grooves, the grating period and the diffraction efficiency within the bounds of our model, we considered a surface relief grating with slanted sinusoidal grooves shape and coefficient $G_1$ defined by Eq. (8). Incorporating $D_{low} = 1.052$ into Eq. (16), and using Eqs. (12)–(15) and (8), we calculated the depth of grooves as a closed form analytical function of the grating period at different Bragg diffraction efficiencies and found the limit of operation for such surface relief gratings, when the incident illumination wavelength is $\lambda = 0.6328 \mu m$, and slant angle $\phi_s = 17^\circ$. The results for TE illumination are presented in Fig. 4. As shown, there are two ranges, where for a specific grating period, two different groove depths would result in the same diffraction efficiency. Also shown, at the right side border of the graph, is an upper bound $A_{s, up}$ that the grating period cannot exceed at a certain Bragg diffraction efficiency and groove depth. This important bound indicates that Bragg efficiency for surface relief gratings can be achieved only by satisfying both the Bragg condition and the bound $A_{s, up}$ determined from Eq. (16).

To experimentally verify our approach, we holographically recorded nearly sinusoidal surface relief gratings with slanted grooves shape, and measured their diffraction efficiency as a function of incident beam angular orientation. The gratings were obtained by recording the interference pattern of two plane waves that were derived from an Argon laser of wavelength $\lambda = 0.363 \mu m$. The recording material was Shipley 1813 photoresist with $n_M = 1.66$ at the readout wavelength of $\lambda = 0.6328 \mu m$, and TE polarization. The experimental arrangement for measuring the diffraction efficiency of the gratings is sche-
matically shown in Fig. 6. It is comprised of a He–Ne laser $L$ with $\lambda = 0.6328 \, \mu m$, a grating $G$ recorded in a photoresist layer which was deposited on a plane glass substrate, a prism $P$, a rotation stage $S$ and a detector $D$. In order to measure the +1st diffraction order, which normally would be trapped by total internal reflection inside the glass substrate, we attached the substrate to the prism with index matching liquid. The prism and grating were placed on the rotation stage, so as to allow variation of incidence angles from 15° to 35° with 1° steps.

The results of the diffraction efficiency measurements, namely the power of +1st diffraction order over the incident power (after accounting for Fresnel reflections on the prism facets), as a function of incidence angle for TE illumination are presented in Fig. 7. Also included are the calculated results obtained both by the analytical calculations of our equivalent grating model and by numerical calculations of the rigorous coupled wave analysis. The analytically calculated maximum diffraction efficiency $\eta_{\text{Bragg}} = 87.5\%$ occurs at a nonzero Bragg incidence angle $\theta_{\text{inc,1}} = 19.5^\circ$. The Bragg angular selectivity is $\Delta \theta_{\text{inc,1}} = 15^\circ$ and spectral selectivity $\Delta \lambda_{1} = 0.2 \, \mu m$ at a threshold level $\eta_{\text{mis}} = 0.9$. As evident, the calculated and experimental results are in good agreement.

In this paper, we developed and experimentally verified an equivalent graded index grating model explaining the Bragg behavior of resonance domain surface relief gratings and providing analytic solutions that can aid in grating design and optimization. Our results reveal that in order to achieve high diffraction efficiency for surface relief gratings certain constraints must be imposed, in addition to the Bragg conditions. These constrains define an upper bound for the grating period at given groove depths.
References