Diffraction efficiency calculations of polarization diffraction gratings with surface relief

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Abstract. In this paper, we evaluate the optical response of a stack of two diffraction gratings of equal one-dimensional periodicity. The first one is a surface-relief grating structure; the second, a volume polarization grating. This model is based on our experimental results from polarization holographic recordings in azopolymer films. We used films of commercially available azopolymer (poly[1-[4-(3-carboxy-4-hydroxyphenylazo) benzenesulfonamido]-1,2-ethanediyl, sodium salt]), shortly denoted as PAZO. During the recording process, a polarization grating in the volume of the material and a relief grating on the film surface are formed simultaneously. In order to evaluate numerically the optical response of this “hybrid” diffraction structure, we used the rigorous coupled-wave approach (RCWA). It yields stable numerical solutions of Maxwell’s vector equations using the algebraic eigenvalue method.

1. Introduction

Various techniques are used to produce diffractive optical elements (DOEs) that modulate and transform light in a predetermined way [1–8]. The DOEs, and surface-relief gratings in particular, are of major interest for applications in quantum electronics, integrated optics, spectroscopy, and holography. Applications include spectral filters, diffractive lenses, antireflection surfaces, beam splitters, beam combiners, beam deflectors, beam shaping elements, laser mirrors, polarization devices, couplers and switches, waveguide couplers, wavelength multiplexers and demultiplexers, etc. [9, 10]. The optical response of a DOE can be controlled by tuning various parameters, such as wavelength, polarization, ratio of the ridge-width to the pitch; the shape of the ridge, the refractive index of the material [11].

The optical response of high-frequency diffraction gratings has to be analyzed by rigorous diffraction approaches for solving the set of Maxwell’s vector equations. Many approximate theories are available for the purpose, the most popular ones using the Kirchhoff approximation [12, 13]. These approaches are simple and easy to apply, but require certain conditions to be met in order to provide accurate results. For example, the wavelength must be much smaller than the grating period, and the

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grating profile must be shallow. However, for a wide range of applications, these conditions are not fulfilled, and the approximations provide inaccurate results.

The analysis of the optical response of the diffraction element depends crucially on a high-precision rigorous modeling of the interaction between light and structure. The mathematical modeling requires the computation of the relation between the incoming and output waves. These quantities are described by a model based on the full set of Maxwell’s vector equations [14, 15]. There exists a variety of different methods for obtaining a numerical solution of the resulting Helmholtz equation. One of the most popular is the rigorous coupled-wave approach (RCWA) [16-18]. Another one is the so-called C method [17]. Boundary value problems for elliptic partial differential equations could also be solved by the finite element method (FEM) [19 - 21].

In RCWA, the grating structure is divided into a number of thin layers (slices) parallel to the surface. Peng et al. [22] first proposed partitioning the grating into thin layers and approximating each layer by a rectangular profile. Each thin grating is then analyzed by using the state-variables method of solving the rigorous coupled-wave equations for that grating. As a result, the efficiencies of all propagating diffraction orders can be estimated.

In the present work, the rigorous coupled-wave approach is used to evaluate the diffraction efficiency of a structure consisting of a scalar surface-relief grating positioned on top of a volume polarization grating.

2. Diffraction structure model and computational implementation of RCWA

Figure 1 presents the “hybrid” diffraction structure considered. The incident plane wave propagates in the superstrate (air) and hits the modulated material (PAZO), which is deposited on the substrate (glass). Two diffraction regions are considered. The first one has a surface–relief grating (SRG) with topological sinusoidal profile \( P \) of period \( d \) along the \( x \)-axis; the second is a region with sinusoidal modulation of the refractive index. Both structures have the same period. It is assumed that there is no shifting between the two gratings.

The \( y \)-axis is perpendicular to the profile plane and the \( z \)-axis is the axis of invariance of the structure (Figure1). The electromagnetic properties of the PAZO material are represented by its complex refractive index [23].

RCWA that we used for evaluation of the diffracted field is based on the algebraic eigen system solution of the of the first-order coupled differential equation. This coupled-wave equation is derived from the full set of Maxwell’s equations. The diffraction structure is split into a set of sublayers (slices), characterized by the material complex refractive index. Within the sublayer, the refractive index is assumed as independent of \( y \) (figure1), i.e. each slice is assumed to have rectangular pieces of modulation within one period of the grating. Using a truncated Fourier expansion of the refractive index, the general coupled-wave equation for the transverse electromagnetic field is solved explicitly for each slice. Solutions at the slice boundaries are evaluated by the continuity of the transverse field components.

Two parameters are of substantial importance: the number of diffraction orders taken in consideration and the number of sublayers used in the diffraction structure representation.

![Figure 1. Diffraction grating notations.](image-url)
3. Results

We consider a recorded polarization grating in azopolymer thin films of commercially available azopolymer (poly[1-[4-(3-carboxy-4-hydroxyphenylazo) benzenesulfonamido]-1,2-ethanediyl, sodium salt]), – PAZO.

The film transmission and reflection are shown in figure 2. The optical constants of PAZO films are obtained using spectrophotometric data, as reported elsewhere [23].

![Figure 2](image1.png)

**Figure 2.** Transmission (left) and reflection (right) of a 300-nm-thick PAZO thin film layer.

During the recording, a polarization grating in the volume of the material and a relief grating on the film surface are formed simultaneously. To investigate how much of the diffraction efficiency is due to the SRG and how much, to the volume polarization grating, we first evaluate the optical response of the thin PAZO film. In this simulation the thickness is \( y_1 = 300 \) nm (figure 1). We then evaluate the diffraction efficiency of the SRG diffraction grating using the RCWA. The SRG is shown in Figure 1. The grating has a pitch \( y_2 = 100 \) nm, \( d = 1000 \) nm and is situated on top of a homogeneous thin film of thickness 300 nm (figure 3). The RCWA is applied to a stack of 12 sublayers with \( \pm 5 \) diffraction orders considered. The homogeneous film is treated as one layer placed on a BK7 substrate.

![Figure 3](image2.png)

**Figure 3.** Wavelength dependence of the calculated transmission diffraction efficiency (DE) of SRG on top of a homogeneous thin film. Zero order – left and first order – right.

Next, we evaluate the diffraction efficiency of a structure consisting of an SRG grating with a pitch \( y_2 = 100 \) nm, and a 300-nm-thick volume grating with sinusoidal modulation. The average refractive index of the azopolymer model grating is set equal to 1.6 and several modulations of \( \Delta n = [0.04, 0.06, 0.08] \) are considered. This diffraction structure model is closest to our experimental diffraction structure. The wavelength dependence of the calculated transmission diffraction efficiency for zero
and +1 diffractive orders of this structure are shown in figure 4. In the RCWA evaluations, we used ± 5 diffraction orders, 12 sublayers for the SRG, 10 sublayers for the volume sinusoidal grating, and BK7 as a substrate.

Figure 4. Wavelength dependence of the calculated transmission diffraction efficiency of an SRG diffraction grating on top of a volume sinusoidal grating. Zero order – left and first order for three different modulations – right.

For our experimentally-recorded grating, at a wavelength of 633 nm we obtained a diffraction efficiency on transmission of first order of 6.1%. For the same wavelength, our model yields a diffraction efficiency of +1 transmission order of 5.45%, and a refractive index modulation slightly above $\Delta n = 0.06$, which agrees with independent measurements of $\Delta n$ of PAZO [24].

4. Conclusions
We evaluated the optical response of a complex diffraction structure consisting of two diffraction gratings of equal one-dimensional periodicity: a thin-film surface-relief grating structure and a volume polarization grating.

The determination of the realistic models and their uncertainties are a challenge, which will require further experiments, mathematical analysis and computational work and post- data processing. As an important next step, we consider solving the inverse problem: estimation of the polarization grating characteristics from the optical response of the overall “hybrid” structure formed in the thin polymer film, having a sound model of the surface grating based on independent experimental data.

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