Modelling of the diffraction efficiency of surface relief gratings with varying spatial frequency, height and shape of the relief

B Blagoeva¹, N Berberova¹, D Nazarova¹, L Nedelchev¹², G Mateev¹, E Stoykova³, E Otsetova-Dudin² and P Sharlandjiev¹

¹ Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, Sofia 1113, Bulgaria
² University of Telecommunications and Post, 1 Acad. St. Mladenov Str., Sofia 1700, Bulgaria

E-mail: blagoeva.bl@iomt.bas.bg

Abstract. An important goal in the development of diffractive optical elements is to achieve high diffraction efficiency. One class of these elements are the surface relief gratings recorded by polarization holography. For recording media, we used azopolymer (poly[1-[4-(3-carboxy-4-hydroxyphenylazo) benzenesulfonamido]-1,2-ethanediyl, sodium salt]), shortly denoted as PAZO. The aim of the present work is to simulate a highly efficient surface relief grating formed in the azopolymer PAZO. The model is based on experimental results already obtained by our group. The tasks of the research are related to the analysis of the diffraction efficiency in the spectral range from 300 nm to 800 nm and for: 1) range of grating spatial frequencies from 1200 ln/mm to 1800 ln/mm, 2) surface relief height varying from 100 nm to 400 nm and 3) different shapes of the formed relief.

1. Introduction

Diffraction gratings are optical elements that are widely used in holography, spectroscopy, quantum electronics and other areas [1–3]. Azopolymers are suitable media for the development of diffractive optical elements (DOE), as they are characterized by high values of the photoinduced anisotropy [4]. By using polarization holographic recording, a diffraction structure is formed in the azopolymer film, which consists of both a surface relief grating (SRG) on the surface of the layer and a polarization holographic grating (PHG) in its volume [5, 6]. In 1996 Barrett et al. prepared a highly efficient SRG, based on trans-cis-trans photosomerization [7].

A large number studies have been conducted, both experimental and theoretical, on diffraction gratings formed by different approaches in azopolymer media [8–13]. It has been experimentally shown that the characteristics of SRG and, accordingly, the optical response of the medium, are influenced by the polarization of the recording beams [14, 15], as well as their power [14]. In previous studies, we experimentally determined the optimal conditions for polarization holographic recording in azopolymer films. We studied the kinetics of the diffraction efficiency (DE) in azopolymer films deposited using different methods, for various spatial frequencies of the gratings, as well as in layers doped with nanoparticles [16, 17]. To obtain a PHG with improved polarization properties, we also proposed a method for suppressing the surface relief, the formation of which deteriorates these properties [18].
The aim of the present study is to model theoretically the optical response of an SRG formed in an azopolymer in the spectral range from 300 nm to 800 nm. To achieve this goal, we take into account the different characteristics of this grating without considering the influence of the PHG. A numerical evaluation of the optical response of an SRG was performed, depending on the height and shape of the relief, as well as the spatial frequency of the grating, using a rigorous coupled-wave approach (RCWA). In this approach, in order to analyze the DE, the structure is divided into thin layers, bringing each layer closer to a rectangular profile [19]. The theoretical approach in this analysis has already been successfully used by us to evaluate the optical response of a diffraction structure consisting of an SRG and a PHG with equal one-dimensional periodicity [20].

2. Optical response estimation approach

2.1. Diffraction structure model

Figure 1 (a) shows the SRG notations used in the present study. Light passes successively through three media with different refractive indices: air, azopolymer and glass. The azopolymer used in the analysis is \((\text{poly}[1-4-(3-carboxy-4-hydroxyphenylazo) benzene sulfonamido]-1,2-ethanediyl, sodium salt])\), shortly denoted as PAZO (Figure 1 (b)), commercially available from Sigma Aldrich. The glass substrate is BK7. As a result of the surface modulation of the azopolymer, diffraction is observed at an angle \(\alpha_n\) between the \(y\)-axis perpendicular to the grid profile and the \(x\)-axis parallel to it, with \(n\) denoting the number of the diffraction order, \(z\) being the axis of invariance of the grating, \(h\), its height; \(\Lambda\) denotes the period of the grating (\(1/\Lambda\) is the spatial frequency) and \(d\), the thickness of the homogenous azopolymer layer.

![Figure 1](image.png)

**Figure 1.** (a) Scheme of surface relief grating and (b) chemical structure of PAZO.

2.2. Computational implementation of RCWA

We model the DE of a surface relief grating using the rigorous diffraction grating efficiency calculation tool in GSolver [21]. To estimate the diffraction orders, the structure is divided into sublayers with rectangular modulation within one grating period. Each sublayer is characterized by the complex refractive index of PAZO, whose values in the spectral range 320–800 nm were calculated by Berberova et al., 2018 [22] based on spectrophotometric data for reflection and transmission. Then, for each sublayer, the total coupled-wave equation for the transverse electromagnetic field is solved using a truncated Fourier expansion of the refractive index; then through the continuity of the transverse components of the field, the solutions within the slice boundaries are evaluated.

3. Results

We theoretically modelled the optical response in the 0 and +1 order of a surface relief grating. The simulation was performed in the case of unpolarized light in the spectral range from 300 nm to 800 nm and normal incidence to the diffraction structure. By setting different grating parameters, we seek the optimal conditions in order to obtain the maximum DE in this azopolymer. Our first task is to determine the spectral dependence of the SRG optical response at three different spatial frequencies of the grating.
– 1200 ln/mm, 1500 ln/mm and 1800 ln/mm (figure 2). The DE was calculated for a grating with sinusoidal modulation and height $h = 100$ nm. The thickness of the homogeneous layer is $d = 300$ nm.

In +1 order, the highest value of DE is observed in the range 400 nm – 700 nm. The modelling result obtained would be useful for future experimental research. In particular, when implementing polarization holographic recording in the PAZO azopolymer, one should select a recording laser with a suitable wavelength, as well as a suitable angle between the recording beams.

In the next step of our numerical modelling, we study the dependence of the optical response on the height of the grating. This dependence is difficult to determine experimentally, as obtaining azopolymer layers of exactly the same thickness is a technical challenge. Therefore, we use a numerical simulation to establish how the height of the relief influences the DE. The calculation is made at fixed parameters $d = 300$ nm, spatial frequency 500 ln/mm and sinusoidal modulation. Four different heights are used – 100 nm, 200 nm, 300 nm and 400 nm (figure 3).

The results show that as the height of the grating increases, the amount of light energy is distributed from zero to higher diffraction orders increases. For the +1 order and a wavelength of 550 nm, the diffraction efficiency increases by 22% approximately when $h$ increases from 100 nm to 400 nm, while the decrease is close to 49% for the zero order.
In the last step of the modelling, we analyze how the shape of the SRG affects the optical response of the medium. Grating profiles with a triangular and a sinusoidal shape with height $h = 100$ nm and spatial frequency 500 ln/mm was used, as well as a homogeneous layer with $d = 300$ nm (figure 4).

The DE of triangular and sinusoidal gratings in the chosen range of characteristics have very similar values – a difference of less than half a percent for the +1 order and less than 1% for the zero order. This result of the numerical modelling indicates that when conducting an experiment under these conditions, one will obtain a similar DE for sinusoidal and triangular relief profile.

4. Conclusion
In the numerical analysis presented, the diffraction is considered of normally incident unpolarized light to a surface relief grating formed in a PAZO azopolymer. The optical response of the diffraction structure depending on the different characteristics of this structure is analyzed using a rigorous coupled-wave approach and is presented in the spectral range from 300 nm to 800 nm. The results show that the highest diffraction efficiency for the +1 order is obtained at a relief height of 400 nm and in the spectral range 400 – 700 nm.

In addition, the dependence is considered of the optical response of the diffraction grating on the shape of the relief. It is shown that for a triangular and a sinusoidal modulation of the relief no significant change in the diffraction efficiency is observed for the orders considered. The results obtained from this numerical modelling would be useful for future experimental studies related to polarization holographic recording in the azopolymer PAZO.

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