Surface relief and polarization gratings for solar concentrators

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Abstract: Transmission gratings that combine a large diffraction angle with a high diffraction efficiency and low angular and wavelength dispersion could be used to collect sunlight in a light guide. In this paper we determine what characteristics a grating should have in order to be useful for such a solar concentrator. To this end we compare the diffractive properties of polarization gratings and classical surface relief gratings. It is found that polarization gratings and classical surface relief gratings have qualitatively comparable diffractive properties as long as their thickness-parameters are within the same regime. The diffraction efficiency of these gratings can be close to 100% for a broad range of incoming angles when the period is large compared to the wavelength of the incoming light. This no longer holds for small-period gratings. For solar concentrators the more easily producible surface relief gratings are preferred over polarization gratings.

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References and links
1. Introduction

Solar energy is a promising response to the world’s growing energy demand. It is clean, reliable and by far the most powerful source of renewable energy. Despite its potential, the use of solar energy is limited due to the high costs associated with semiconductor-based photovoltaic elements. In order to make solar energy economically competitive and suitable for large-scale use, these costs must be cut back. One way to achieve this is by reducing the required area of expensive solar cells using a concentrator system that focuses incoming sunlight onto a small area of solar cells. Usually, such concentrator systems consist of lenses and mirrors [1, 2]. This results in large, heavy systems that need to track the movement of the sun and are still relatively expensive.

Alternatively, a plastic light guide can be used as an inexpensive, flat and lightweight solar concentrator. Sunlight is coupled into this light guide and gets trapped inside due to total internal reflection (TIR). The light is then guided towards a small solar cell via TIR. Producing a solar concentrator in this way requires structures that efficiently couple sunlight into the light guide. Several ways to do so have been studied and they all have disadvantages. Refractive structures are bulky. The use of scattering elements always leads to limited efficiency. Luminescent solar concentrators [3], in which a fluorescent dye absorbs sunlight and re-emits it into TIR, suffer from significant losses via the top and the bottom of the light guide [4] and by re-absorption at the dye molecules.

In this paper we study diffraction gratings as an alternative method for coupling sunlight into a light guide [5, 6]. Diffraction gratings are compact and relatively inexpensive to make. When applied on top of a light guide they diffract the incoming sunlight into multiple directions. If the diffraction angle of a specific order is larger than the critical angle of the light guide that part of the transmitted light gets coupled into TIR. For solar concentration this in-coupling mechanism should be made efficient. To this end, the gratings should combine a number of properties. First of all, they should have a high diffraction efficiency (i.e. a low 0th order, since this constitutes loss). Secondly, a relatively small grating period (or pitch size) is required in order to achieve a diffraction angle larger than the critical angle of the light guide material. In order to avoid
tracking and to capture diffuse sunlight, the grating should be as insensitive to the angle of incidence as possible. Finally, since we are dealing with sunlight, unpolarized light and a broad spectrum of wavelengths need to be taken into account.

In this study we assess two types of gratings: classical surface relief gratings and liquid-crystal-based polarization gratings. Both can be produced using holographic techniques. We compare their diffractive properties, especially the possibility to minimize the 0th order and the angular dependence of the diffraction efficiency, and determine to what extent they meet the above mentioned requirements. From this study we determine which grating characteristics result in high in-coupling efficiencies. Finally, we consider whether the gratings can be made with the required parameters.

2. Holographic production of gratings

Diffraction gratings can be produced using techniques like holography, lithography and e-beam. Although most considerations are independent of the production techniques, the gratings considered in this paper are produced holographically. Holographic production can be done relatively fast and gives easy control over grating parameters. Two coherent incoming beams generate an interference pattern, which is recorded in a photosensitive material. The period $\Lambda$ of the interference pattern is given by $\Lambda = \lambda_{\text{rec.}} / (2 \sin \theta_{\text{rec.}})$, where $\lambda_{\text{rec.}}$ is the wavelength of the two recording beams and $\theta_{\text{rec.}}$ the half angle separating them. We distinguish two forms of holography: normal intensity holography, resulting in surface relief gratings and polarization holography, with a periodic variation of the polarization and resulting in polarization gratings.

For normal intensity holography the two incoming beams have equal s-polarization. Their interference pattern is constant in polarization, equal to the polarization of the two generating beams, and fluctuates in intensity. A photosensitive material (or photoresist) can record the various high and low intensity areas. After a development step only the intensely illuminated (negative photoresist) or only the non-intensely illuminated (positive photoresist) areas remain and a surface relief grating is obtained. In this paper the non-linear negative photoresist SU-8 is used [7, 8].

For polarization holography the two incoming beams have orthogonal polarizations. This results in an interference pattern with (in the paraxial approximation for small recording angle $\theta_{\text{rec.}}$), constant intensity, but fluctuating polarization. For the production of liquid-crystal-based polarization gratings two orthogonal circularly polarized beams are used and the resulting interference pattern is (again in the paraxial approximation) linear everywhere. The direction of this linearity changes over a period from s-polarized to p and back to s [9, 10]. This pattern can be recorded in a linear photo-polymerizable polymer (LPP). When LPP is illuminated with UV light it aligns in the direction of the polarization, thereby recording the polarization holographic pattern. It is then used as an alignment layer for a nematic liquid crystal. When the angle between the recording beams becomes larger, corresponding to smaller grating periods, the paraxial approximation no longer holds. Then the interference pattern is not completely constant in intensity and its polarization is slightly elliptical [10]. In this case it is assumed that the liquid crystal aligns with the long axis of this ellipse.

3. Surface relief gratings

Surface relief gratings are interesting for large scale applications, since they can be reproduced relatively easy from a master. Classically, isotropic gratings can be categorized as either thick or thin [11]. Thick gratings show Bragg diffraction. Their diffraction efficiency can be approximated analytically using Kogelnik’s coupled wave theory [12], which is valid close to the Bragg angle. Thin isotropic gratings show Raman-Nath diffraction. They are classically treated with scalar diffraction theory and their far field diffraction efficiencies are approximated using the
Fraunhofer approximation [13]. When a beam is diffracted by a thin grating, the Fraunhofer approximation for the far field $E_m$ of the $m^{th}$ diffracted order can be written as:

$$E_m = \frac{1}{\Lambda} \int_0^{\Lambda} E_{in} \exp \left[ -2\pi i (mx/\Lambda + dn(x)/\lambda) \right] dx,$$

where $\Lambda$ is the grating period, $E_{in}$ the (scalar) field of the incoming beam, $\lambda$ the incoming wavelength, $d$ the thickness of the layer constituting the grating and $n(x)$ the refractive index modulation. For surface relief gratings $n(x)$ corresponds to the height profile of the surface relief. Note that Eq. (1) holds at normal incidence, for $d \downarrow 0$, in which limit volume gratings and a surface relief gratings can be treated equally and assuming that the paraxial approximation holds. For a number of profiles $n(x)$, the integral in Eq. (1) can be calculated analytically and expressions for the diffraction efficiencies $\eta_m = |E_m|^2/|E_{in}|^2$ are obtained. A sinusoidal profile leads to the well-known Raman-Nath expression [14].

The efficiency of the $m^{th}$ order is given by:

$$\eta_m = J_m^2(\pi\Delta n/\lambda),$$

where $J_m$ are ordinary Bessel functions of the first kind and $\Delta n$ is the maximal refractive index difference within the grating ($\Delta n = n_{\text{resist}} - n_{\text{air}}$ for surface relief gratings). The diffraction efficiency for a rectangular surface relief (or binary volume) grating can be calculated as:

$$\eta_m = \frac{\sin^2(m\pi/2)}{\cos^2(\pi \Delta n/\lambda - m\pi/2)}$$

$$= \begin{cases} 
\cos^2(\pi d\Delta n/\lambda), & \text{for } m = 0; \\
4/(m\pi)^2 \sin^2(\pi d\Delta n/\lambda), & \text{for } m = 2k + 1; \\
0, & \text{for } m = 2k, k \neq 0,
\end{cases}$$

where $k \in \mathbb{Z}$. A triangular profile leads to

$$\eta_m = \frac{1}{4} [\sin(\pi \Delta n/\lambda - m\pi/2) + (-1)^m \sin(\pi \Delta n/\lambda - m\pi/2)]^2.$$

In order to categorize gratings as either thick or thin for finite values of $d$, one may look for a parameter that indicates whether the analytical approximations for Bragg or Raman-Nath diffraction are reasonable. This is done by comparing $d$ and the wavelength $\lambda$ with $\Delta n$ and/or the average index of refraction $n_{\text{av}}$ and the grating period $\Lambda$. Most often, the Klein parameter [15],

$$Q = \frac{2\pi d\lambda}{n_{\text{av}}\Lambda^2},$$

is used and the grating is considered thin when $Q < 1$ and thick when $Q > 10$. Another frequently used parameter is [14]:

$$\rho = \frac{2\lambda^2}{n_{\text{av}}\Delta n\Lambda^3},$$

for which $\rho < 1$ is considered as thin and $\rho \gg 1$ as thick. Other parameters, often modifications of $Q$ or $\rho$, can also be used. Also, a different parameter may be chosen for different regimes. The definition of the regimes may depend on the situation and the chosen criterium. Consequently, the distinctive parameter and the terminology can be confusing.

Despite this ambiguity, one can always assure that a grating can be considered thin by choosing the pitch size large enough. For low values of $d$ the diffraction efficiency is less sensitive to the incoming angle and wavelength [11] and to relative changes in $d$. Therefore, $d$ should be of the same order of magnitude as the first value that minimizes $\eta_0$ in order to control the
diffraction efficiency. Since experimental surface relief profiles may resemble sinusoidal or rectangular shapes, this value of \( d \) will be around:

\[
d = \begin{cases} 
  \frac{2.4\lambda}{(\pi\Delta n)} & \text{(sinusoidal profile);} \\
  \frac{\lambda}{(2\Delta n)} & \text{(rectangular profile)},
\end{cases}
\]

where we set \( \eta_0 = 0 \) in Eq. (2) and Eq. (3). Therefore, \( \Lambda \gg \lambda \) leads to \( Q, \rho \ll 1 \) for reasonable values of \( n_{av} \) and \( \Delta n \).

For gratings that are neither thick nor thin and also for angles of incidence that significantly deviate from 0° or from the Bragg angle no analytical approximations exist and one has to reside to exact numerical methods like Rigorous Coupled Wave Analysis (RCWA) [16, 17], the Finite-Difference Time-Domain method (FDTD) [18] or the Finite Element Method (FEM) [19] to determine the diffraction efficiencies. For surface relief gratings we used the commercially available software GSolver [20], which is based on RCWA.

### 3.1. Large-period surface relief gratings

In this section we consider surface relief gratings produced in SU-8 (\( n_{SU-8} = 1.59 \)) with a large pitch size compared to the incoming wavelength: \( \Lambda = 15 \mu m \) and \( \lambda = 633nm \), assuring that the gratings can be considered as thin.

#### 3.1.1. Normal incidence

![Image of calculated diffraction efficiency as a function of the height \( d \) at normal incidence for a thin surface relief grating in SU-8: \( \Lambda = 15 \mu m, \lambda = 633nm, s\)-polarization. Solid lines show the RCWA results, dotted lines the corresponding Fraunhofer approximation (FA). (a) Sinusoidal surface relief. (b) Rectangular surface relief.](image)

Since the Fraunhofer approximation is only exact in the limit \( d \downarrow 0 \), we used RCWA to study the influence of the shape of the surface relief profile and of the thickness \( d \) and to see to what extend Eq. (2) and Eq. (3) still hold as \( d \) increases. The simulations assume that the gratings were produced on top of a light guide with \( n_{out} = 1.6 \) and that the incoming light is \( s\)-polarized. The resulting \( 0^{th} \) and \( \pm 1^{st} \) orders are plotted in Fig. 1 (solid lines), together with the corresponding Fraunhofer expressions (dashed lines). The Fraunhofer approximation is followed closely for low values of \( d \). For higher values of \( d \) the simulated results start to deviate from the analytical approximations. This is most clearly visible for the rectangular grating. Its \( 0^{th} \) order shows a seemingly exponential damping with increasing \( d \), which is mainly due to the fact that higher even orders become non-zero.
3.1.2. Angular dependence

To study the angular dependence of a thin surface relief grating with RCWA, we again assumed $\Lambda = 15 \mu m$, $\lambda = 633$ nm and s-polarization. The thickness $d$ was chosen at the first minimum of $\eta_0$ in Fig. 1 in order to maximize the diffraction efficiency and to minimize the angular dependence: $d = 2.44/(\pi \Delta n) = 821$ nm for the sinusoidal grating and $d = \lambda/(2\Delta n) = 536$ nm for the rectangular grating. The results are plotted in Fig. 2. It is observed that the sinusoidal grating has significantly higher $\pm 2$nd orders compared to the rectangular grating, resulting in lower $\pm 1$st orders at low angles of incidence and a lower 0th order at high angles of incidence. More importantly, as the angle of incidence is increased from $\theta = 0$ the diffraction efficiency initially decreases only slowly. The 0th order remains less than 10% for angles of incidence as high as $55^\circ$ and $45^\circ$ for a sinusoidal and a rectangular grating respectively, which seems promising for our application.

![Fig. 2](image)

3.1.3. Experimental

Next to these simulations, we experimentally verified the low 0th order and the wide angular acceptance for a surface relief grating produced in SU-8. To promote adhesion of the grating to the substrate, first a thin layer of SU-8 was spin coated on a glass substrate (SU-8 2000 series, MicroChem). After evaporating the solvent the sample was flood exposed and baked at 95°C to obtain a fully cross linked layer. Next the sample was treated with UV-Ozone for 15 minutes and a second layer for holographic recording was spin coated from a 29wt% solution of SU-8 at 3000 rpm for 30 seconds. After evaporation of the solvent the sample was exposed in an intensity holographic setup with a periodicity of approximately $15 \mu m$ using an $\text{Ar}^+\text{-laser}$ operated at the 351 nm UV-line with a dose of approximately 14 mJ/cm². The sample was then baked at 95°C, etched using appropriate developer solvent (MicroChem) and finally rinsed in isopropanol to obtain a surface relief grating. Heating of the sample was always done gradually and afterwards it was allowed to cool to room temperature. Using confocal microscopy, the pitch size $\Lambda$ and grating thickness $d$ were measured to be approximately $15.6 \mu m$ and $0.6 \mu m$ (see Fig. 3).

As a reading beam, an s-polarized 633 nm HeNe-laser was used and the diffraction efficiencies of the 0th, $\pm 1$st and $\pm 2$nd orders were measured as a function of the angle of incidence.
The results are plotted in Fig. 4a. Next, a profile for this particular grating was derived from the confocal microscopy images (Fig 3) and used to calculate the angular dependence using RCWA as well. The RCWA results are shown in Fig. 4b. The measured and simulated results are in good agreement. It is observed that the 0th order indeed remains low for a wide range of incoming angles. Most interestingly, the efficiencies of the ±1st and ±2nd orders are high and relatively insensitive to the angle of incidence. The behavior of the diffraction efficiencies is in between those expected for a sinusoidal and a rectangular grating (c.f. Fig 2), as to be expected, since the profile observed in Fig. 3 is neither a perfect rectangle, nor a perfect sine.

3.2. Small-period surface relief gratings

Let us now determine how gratings for in-coupling into a light guide can be categorized. The refractive index modulation is fixed by the choice of materials. In our case, a surface relief grating in SU-8 with \( n_{\text{SU-8}} = 1.59 \) and \( n_{\text{air}} = 1 \), we obtain \( n_{\text{avg}} = 1.295 \) and \( \Delta n = 0.59 \). The grating period is limited by the requirement that light should be coupled into TIR. From the grating equation it can be seen that at normal incidence a grating period equal to the wavelength
of the incoming light results in a diffraction angle for the first orders equal to the critical angle of the light guide, irrespective of the grating and light guide materials: \(m\lambda / \Lambda = n_{\text{out}} \sin(\theta_m)\) gives \(\theta_{\pm 1} = \pm \arcsin(1/n_{\text{out}}) = \pm \theta_{\text{crit}}\). In practice, \(\Lambda \lesssim \lambda\) is taken to obtain a small range of angles of incidence that is coupled into TIR. For non-thin gratings the lowest value of \(d\) that minimizes \(\eta_0\) should be found numerically. However, in general it will be smaller than for thin gratings and using Eq. (8) as an upper bound it can be estimated as \(d \lesssim \Lambda \lesssim \lambda\). Inserting these estimates in the definition for \(Q\) or \(\rho\), we find that gratings for in-coupling cannot be considered as either thick or thin, regardless of the defining thickness parameter. Therefore we use RCWA again in this section [20].

The possibility to design a grating with vanishing 0th order and a wide angular acceptance, as was observed in Section 3.1 for large-period surface relief gratings, is interesting for in-coupling applications. In the remainder of this section we will consider to what extend these properties still hold for surface relief gratings with \(\Lambda \lesssim \lambda\), suitable for coupling light into TIR. This is done assuming a grating with a sinusoidal or a rectangular profile in SU-8 \(n_{\text{SU8}} = 1.59\) with a period \(\Lambda = 600\,\text{nm}\) and applied on a light guide with \(n_{\text{out}} = 1.6\) for s-polarized light with wavelength \(\lambda = 633\,\text{nm}\).

### 3.2.1. Normal incidence

First the thickness \(d\) is varied at normal incidence. The result is plotted in figure 5. It is observed that for these non-thin gratings there is no value of \(d\) for which the \(\eta_0\) vanishes. The diffraction efficiency still shows an oscillation with varying \(d\), albeit not as smooth as for the grating in Fig. 1 and with a smaller periodicity.

![Fig. 5. Calculated (RCWA) diffraction efficiency as a function of the height \(d\) at normal incidence for a non-thin surface relief grating in SU-8: \(\Lambda = 600\,\text{nm}, \lambda = 633\,\text{nm}, \) s-polarization. (a) Sinusoidal surface relief. (b) Rectangular surface relief.](image)

### 3.2.2. Angular dependence

Analogous to the case of the thin \(\Lambda = 15\,\mu\text{m}\) grating, we studied the angular dependence of a non-thin \(\Lambda = 600\,\text{nm}\) surface relief grating. The thickness \(d\) was chosen at the first maximum of \(\eta_{\pm 1}\) in Fig. 5: \(d = 410\,\text{nm}\) for a sinusoidal grating and \(d = 351\,\text{nm}\) for a rectangular grating. The results are plotted in Fig. 6. The rectangular profile performs slightly better at small angles of incidence and the sinusoidal grating has a larger \(-1^{\text{st}}\) and a smaller \(-2^{\text{nd}}\) order at high angles of incidence. However, the differences are not as profound as in the case of thin gratings (c.f.
Fig. 2) and we conclude that the shape of the relief profile is of minor influence on the angular dependence for non-thin gratings, as long as the thickness \( d \) is adjusted appropriately.

![Diffraction efficiency for sinusoidal and rectangular surface relief grating](image)

Fig. 6. Calculated (RCWA) diffraction efficiency as a function of the angle of incidence for a non-thin surface relief grating in SU-8: \( \Lambda = 600 \text{ nm} \), \( \lambda = 633 \text{ nm} \), s-polarization. Left panel: sinusoidal surface relief with \( d = 410 \text{ nm} \). Right panel: rectangular surface relief with \( d = 351 \text{ nm} \).

More importantly, comparing Fig. 6 and Fig. 2, we see that the diffraction efficiency of the non-thin gratings is much more sensitive to the angle of incidence. Both the \(+1^{\text{st}}\) and \(-1^{\text{st}}\) order drop quickly as \( \theta \) is increased, resulting in a high \( 0^{\text{th}} \) order. It can be concluded that insensitivity to the angle of incidence is a property for thin surface relief gratings, and does not hold for the small-period, non-thin case.

3.2.3. Experimental

We experimentally verified the above findings for a non-thin grating produced in SU-8. Fabrication was similar to the grating with \( \Lambda \approx 15.6 \mu \text{m} \). The recording layer was spin coated on a glass substrate from a 29wt% solution at 3000 rpm for 30 seconds and exposed in a holographic setup with a dose of approximately 10mJ/cm\(^2\). After development the grating shown in Fig. 7 was obtained. Using scanning electron microscopy (SEM) its pitch \( \Lambda \) and thickness \( d \) were measured to be approximately 0.59\( \mu \text{m} \) and 0.4\( \mu \text{m} \), respectively. Again, a HeNe-laser

![SEM images of a non-thin surface relief grating in SU-8](image)

Fig. 7. SEM images of a non-thin surface relief grating in SU-8: \( \Lambda \approx 590 \text{ nm} \), \( d \approx 0.4 \mu \text{m} \).
(\(\lambda = 633\text{ nm}, \text{s-polarization}\)) was used as a reading beam. To prevent the diffracted orders from being totally internally reflected within the substrate, the sample was placed in the center of a PMMA hemisphere and brought into optical contact using an index matching liquid, assuring that the diffracted beams encounter the PMMA-air interface at normal incidence. Subsequently, the diffraction efficiencies were measured for various angles of incidence. The results are plotted in Fig. 8a. From the SEM analysis a grating profile was extracted and used to calculate the diffraction efficiency as a function of the angle of incidence for this sample with RCWA (Fig. 8b). The drop in \(\eta_{-1}\) around \(\theta = 5^\circ\) and the rise in \(\eta_{-2}\) for large angles of incidence are less profound in the measurement, but in general the measurement and the RCWA result are in good agreement. Comparing Fig. 8 and Fig. 6, we observe that the angular dependence of the experimental small-period grating is qualitatively as expected. More importantly, when compared to the large-period grating (c.f. Fig. 4), we observe that for this small-period grating the 0th order is indeed larger at \(\theta = 0^\circ\) and shows an additional sharp rise when \(\theta\) is increased, resulting in low in-coupling efficiencies.

![Fig. 8. Measured (a) and calculated (RCWA) (b) diffraction efficiency as a function of the angle of incidence for a non-thin surface relief grating in SU-8: \(\Lambda = 600\text{ nm}, d \approx 0.4\mu\text{m}\), \(\lambda = 633\text{ nm}, \text{s-polarization}\).](image)

3.2.4. High-\(\Delta n\) small-period surface relief gratings

From the previous paragraph it follows that with small-period surface relief gratings produced in SU-8 only light from a very limited range of incoming angles around \(\theta = 0^\circ\) can be coupled efficiently into TIR due to the poor angular dependence of non-thin gratings and their non-vanishing 0th order. According to the parameters \(Q\) and \(\rho\) (Eq. (6) and Eq. (7) respectively) the thickness-parameters of a surface relief grating can also be decreased using a material with higher refractive index, thus increasing \(n_{av}\) and \(\Delta n\). Therefore, we performed simulations for surface relief gratings produced in a material with refractive index \(n = 2.49\) (e.g. titanium dioxide), \(\Lambda = 600\text{ nm}, \lambda = 633\text{ nm}\) and s-polarized light. Fig. 9 shows the diffraction efficiency as a function of the height \(d\) at normal incidence for a sinusoidal and a rectangular profile. It is observed that, using this high refractive index, it is possible to choose a value for \(d\) for which \(\eta_0\) vanishes. Also the angular dependence is improved compared to surface relief gratings produced in SU-8, as can be seen in Fig. 10. The 0th order is low for a longer range of incoming angles. The +1st order remains high until it becomes evanescent, especially for the rectangular profile, and is diffracted into TIR over this whole range. Note that this shows that a vanishing 0th order and a good angular acceptance are a consequence of a low thickness-parameter and
not just a paraxial effect, as would still be possible based on only Sections 3.1 and 3.2. The gratings studied in Fig. 10 are on the edge of being thin or non-thin: \( Q = 1.66 \) and \( Q = 1.83 \) for rectangular and sinusoidal respectively and \( \rho = 0.86 \) for both.

Fig. 9. Calculated (RCWA) diffraction efficiency as a function of the height \( d \) at normal incidence for a small-period surface relief grating in titanium dioxide: \( n = 2.49, \Lambda = 600 \text{ nm}, \lambda = 633 \text{ nm}, s \)-polarization. Left panel: sinusoidal surface relief. Right panel: rectangular surface relief.

Fig. 10. Calculated (RCWA) diffraction efficiency as a function of the angle of incidence for \( s \)-polarized light for a small-period surface relief grating in titanium dioxide: \( n = 2.49, \Lambda = 600 \text{ nm}, \lambda = 633 \text{ nm} \). (a) Sinusoidal surface relief with \( d = 289 \text{ nm} \). (b) Rectangular surface relief with \( d = 262 \text{ nm} \).

4. Polarization gratings

Liquid crystal-based polarization gratings can be made with 100% diffraction efficiency. Furthermore, previous simulations indicated that their diffraction efficiency is relatively insensitive to the angle of incidence [10]. Based on these arguments, they seem to be a good choice as gratings for solar concentrators. However, the theoretical 100% diffraction efficiency was found in the paraxial approximation, which is valid for the large pitch sizes that are usually considered
in literature. In the paraxial approximation the diffraction efficiency of polarization gratings is
given by [9, 21, 22]:

\[
\eta_0 = \cos^2\left(\frac{\pi \Delta n d}{\lambda}\right),
\]

(9)

\[
\eta_{\pm 1} = \frac{1 \pm S_3'}{2} \sin^2\left(\frac{\pi \Delta n d}{\lambda}\right),
\]

(10)

where \(S_3'\) is the normalized Stokes parameter of the incoming light that characterizes the
circularity and \(\Delta n\) now denotes the birefringence of the nematic liquid crystal. \(\eta_0\) thus vanishes
when the thickness and wavelength are related as \(d = \lambda / 2\Delta n\).

The wide angular acceptance was so far only found in simulations done for relatively large
pitch sizes. With the analysis of surface relief gratings from Section 3 in mind, we may wonder
whether these properties are not just a consequence of the fact that the polarization gratings
that were studied could be considered as thin. In this section we verify the good angular accep-
tance that was found numerically by Xu et al. [10] for large-period polarization gratings experi-
mentally and we study to what extend it still holds for small periods, useful for in-coupling
applications (\(\Lambda \sim \lambda\)).

There is some work done on categorizing polarization gratings as thick and thin. Oh and
Escuti [23] find that the parameter \(\rho\) given by Eq. (7) and not the Klein parameter \(Q\) given
by Eq. (6) should be used for polarization gratings. This is of limited use to us here, since in
their study of the parameter \(\rho\), \(d\) is fixed at \(d = \lambda / 2\Delta n\) (assuming this minimizes \(\eta_0\), which is
only true as long as (9) holds), while \(d\) is a variable in the Klein parameter and not fixed in its
analysis. We note that, apart from a prefactor \(\pi / 2\), the Klein parameter \(Q\) is identical to \(\rho\) when
the relation \(d = \lambda / 2\Delta n\) is substituted into Eq. (6).

It is not our goal here to determine which parameter should be used to categorize polariza-
tion gratings. Our point of view is that there is no reason to assume that classifying polarization
gratings would be any different from classifying surface relief gratings. The fundamental dif-
fERENCE of polarization gratings, compared to surface relief gratings, is the use of birefringent
materials and therefore there should be no major differences in diffractive properties that can-
not be attributed to polarization effects. Thus, we assume that the terminology \textit{thick} and \textit{thin}
should be used in the same manner as for surface relief gratings. Again, this terminology and
the distinctive parameter may be confusing and could depend on the situation. Just as for sur-
face relief gratings, for reasonable values of \(d\) (same order of magnitude as \(d = \lambda / 2\Delta n\)) and
\(n_{av}\) and \(\Delta n\) (typically \(n_{av} \simeq 1.6\) and \(\Delta n \simeq 0.2\)) a polarization gratings will be thin when \(\Lambda \gg \lambda\)
and polarization gratings for in-coupling will be neither thick nor thin.

4.1. Large-period polarization gratings

For a thorough numerical study of the thickness and angular dependence of thin polarization
gratings we refer to Xu et el. [10]. Using FEM they verified Eq. (9) and showed that the diffrac-
tion efficiency can be high for a broad range of incoming angles for thin polarization gratings.
Here we verify this experimentally. In order to compare the results with the surface relief grat-
ing in Section 3.1, we used \(\Lambda = 15 \mu m\), \(\lambda = 633\, \text{nm}\) and s-polarization.

4.1.1. Experimental

To obtain the polarization grating, LPP (Rolic) was spin coated on two glass substrates, which
were then arranged as a cell with a spacing \(d \approx 3 \mu m\). This cell was exposed in a polarization
holographic setup with a periodicity of 15 \(\mu m\) using the 351 nm-line of an Ar\(^+\)-laser. Finally,
the cell was filled with a nematic liquid crystal with \(n_e = 1.6134\) and \(n_o = 1.5010\) (ZLI-2222-
000, Merck), which aligned with the fluctuating direction of the LPP (see Fig. 11a).
Fig. 11. Polarization microscopy images of thin polarization gratings. The polarization grating in (a) is made with ZLI-2222-000 (Merck), for which the difference in elastic constants $K_3 - K_1$ is small. The grating in (b) is made using E7 (Merck), for which $K_3 - K_1$ is large. In (b) we observe a periodically recurring misalignment. The indicated director in picture can be $\Lambda/2$ off.

Fig. 12. Measured diffraction efficiency as a function of the angle of incidence for an experimental thin polarization grating: $n_e = 1.6134, n_o = 1.5010, \Lambda \approx 15 \mu m, d \approx 3 \mu m, \lambda = 633 nm$, s-polarized light. As a reading beam, an s-polarized 633 nm HeNe-laser was used and the efficiencies of the 0th, ±1st and ±2nd orders were measured for various angles of incidence. The result is plotted in Fig. 12. The total efficiency does not add up to 100%, mainly due to reflections and scattering inside the sample (as $\eta_{\pm2}$ were small). Indeed, a high diffraction efficiency for $m = \pm1$ is observed over a broad range of incoming angles and $\eta_0$ is remarkably low over the whole range. For high $\theta$ it is less than found by Xu et al. for this situation (Ref. [10], Fig. 9b), which is due to the fact that we studied a larger pitch size (Ref. [10] shows that a smaller thickness-parameter results in lower $\eta_0$ at high $\theta$) and to reflection at the glass-air interface. The result in Fig. 12 therefore agrees well with numerical results.

4.2. Small-period polarization gratings

Xu et al. also studied small-period polarization gratings at normal incidence (Ref. [10], Fig. 11) and showed that decreasing the pitch size results in lower diffraction efficiencies. In their study, the highest thickness-parameter occurs for a grating with $\Lambda = 678$ nm, $\Delta n \approx 0.2$ at $\lambda = 633$ nm, which results in a minimum for the 0th order of $\eta_0 \approx 0.7$ around $d \approx 875$ nm. We used the same numerical method, FEM [19], to study the angular dependence of this polarization gratings. The calculated diffraction efficiency is shown in Fig. 13a as a function of the angle of incidence. A low diffraction efficiency is observed for all angles of incidence. Like for surface relief gratings,
the relative changes in the diffraction efficiencies upon increasing $\theta$ are larger for this small-period grating than for the large-period grating (c.f. Fig 12). The wide angular acceptance, as found for thin polarization gratings, does not hold for the non-thin case.

4.2.1. High-$\Delta n$ small-period polarization gratings

Comparing Fig. 13a and Fig. 6 we observe that the diffraction efficiency of the small-period polarization grating is also significantly lower than that of the small-period surface relief grating. This is because the birefringence of the liquid crystal is only $\Delta n = 0.2$, which is a realistic value, but much lower than the difference between high index ($n_{SU-8} = 1.59$) and low index ($n_{air} = 1$) regions in an SU-8 relief grating. To show that the angular dependence of polarization gratings is comparable to that of surface relief gratings if their parameters are comparable, we performed an additional FEM simulation for a hypothetical liquid crystal having a $\Delta n$ equal to the SU-8 relief grating and a similar thickness: $n_e = 1.59, n_o = 1$ and $d = 323$ nm. The resulting diffraction efficiency is plotted in Fig. 13b, as a function of the angle of incidence. The higher birefringence results in higher diffraction efficiencies, around 30%, for the $\pm 1^{st}$ orders close to normal incidence, which drops with increasing angle of incidence. This behavior is qualitatively comparable to that of the surface relief gratings in Fig. 6.

4.2.2. Production of small-period polarization gratings

In order to maximize the diffraction efficiency of a polarization grating a certain thickness is required: $d = \lambda / 2\Delta n$ when Eq. (9) holds and a smaller $d$, to be found numerically, when Eq. (9) no longer holds. In this section we address the question whether this thickness is practically realizable for a small-period polarization grating. One has to determine whether the nematic liquid crystal will align according to the director

$$n = (\cos \theta_n \cos \phi_n, \cos \theta_n \sin \phi_n, \sin \theta_n) = (\cos(\pi x/\Lambda), \sin(\pi x/\Lambda), 0),$$

as imposed by the LPP-alignment layers. This means that its corresponding free energy density, given by [24]

$$F = \frac{1}{2} \left( \frac{\pi}{\Lambda} \right)^2 \left[ K_1 \sin^2(\pi x/\Lambda) + K_3 \cos^2(\pi x/\Lambda) \right],$$

Fig. 13. Calculated (FEM) diffraction efficiency as a function of the angle of incidence for a non-thin polarization grating ($\lambda = 633$ nm, s-polarized light). (a) Polarization grating with $\Lambda = 678$ nm, $d = 875$ nm and $\Delta n = 0.2$. (b) Polarization grating with $\Lambda = 600$ nm, $d = 323$ nm and $\Delta n = 0.59$. 

$$m = 0$$

$$m = -1$$

$$m = 1$$

$$\theta (°)$$

$$\eta_m$$

$$\Delta n = 0.2$$

$$\Lambda = 678 \text{ nm}$$

$$d = 875 \text{ nm}$$

$$\Delta n = 0.59$$

$$\Lambda = 600 \text{ nm}$$

$$d = 323 \text{ nm}$$

$$\Delta n = 0.59.$$
where $K_1$, $K_2$ and $K_3$ are the elastic constants representing splay, twist and bend respectively, should minimize the total free energy for the desired pitch $\Lambda$ and thickness $d$. When Eq. (12) does not minimize the total free energy the alignment gets distorted (i.e. $\theta_n$ becomes non-zero). Note that a non-zero $\theta_n$ introduces terms in the free energy density proportional to $K_2$. In Fig. 11b, which shows a polarization micrograph for a grating made using another liquid crystal (E7, Merck), some distortions in the alignment pattern arise that are not present in Fig. 11a. An explanation could be that the $F$ as given by Eq. (12) fluctuates more with $x$ when the difference between $K_1$ and $K_3$ is larger. This makes some regions energetically less favorable than others and there the alignment might get distorted more easily. Intuitively, one may therefore assume that liquid crystals with large $K_2$ and small $K_3 - K_1$ result more stable polarization gratings.

By assuming a small distortion $\theta_n$ depending only on $z$ (where $z$ is the coordinate normal to the grating plane), it can be shown analytically that the director in Eq. (11) does not correspond to a minimum of the total free energy when the thickness $d$ exceeds a certain critical value $d_c$ [25, 26]. For $d > d_c$ the alignment will get distorted for every $x$. This critical thickness is a function of the elastic constants, but also of the period: $\Lambda/(2K_3/K_1 - K_2/K_1)^{1/2} \leq d_c \leq \Lambda$ according to Ref. [26]. Requiring $d \leq \Lambda/2$ is often taken as a practical rule of thumb. As a result, a polarization grating with a small period $\Lambda$ is only stable when its thickness becomes very small. Apart from being difficult to realize practically, $d_c$ becomes smaller than the thickness required to maximize the diffraction efficiency for small-period polarization gratings and realistic values of $\Delta n$. Polarization gratings with $d \approx \Lambda \lesssim \lambda$ can therefore not be experimentally realized.

5. Discussion

Comparing the results obtained in Section 3 and Section 4 we observe several similarities between polarization gratings and surface relief gratings. First of all, both polarization gratings and surface relief gratings can be made with vanishing $0^{th}$ order as long as they can be considered thin. When this holds, the diffraction efficiencies vary slowly with varying angle of incidence. The similarities between rectangular surface relief gratings and polarization gratings are remarkable. In the paraxial approximation the only difference is the presence of odd orders higher than $\pm 1$ for rectangular surface relief gratings (c.f. Eq. (3) and Eq. (9)) and these higher orders can be very low, especially for low values of $d$. Also the angular dependence (Fig 2b and Fig. 12) is similar, especially for the $\pm 1$ orders.

The changes upon going from large-period, thin gratings to small period, non-thin gratings are comparable for surface relief and polarization gratings. For common values of $\Delta n$, it is no longer possible to obtain a vanishing $0^{th}$ order and the diffraction efficiency drops beyond from normal incidence. Better performance is obtained for small values of $\Lambda/\lambda$ when $\Delta n$ is larger, which makes the thickness-parameters smaller. High values of $\Delta n$ are more easily obtained for surface relief gratings. Again, the angular dependence (Fig. 6 and Fig. 13b) is qualitatively comparable.

The diffractive properties of polarization gratings are usually presented as a result of the specific alignment of the liquid crystal. This obviously holds for their polarization dependence, but for properties that do not result from birefringence the behavior is not fundamentally different from surface relief gratings. The commonly mentioned low $0^{th}$ order and the insensitivity to the angle of incidence are a mere consequence of the fact that polarization gratings with $\Lambda \gg \lambda$ were considered. In this respect they behave similarly as surface relief gratings as long as their parameters are comparable. For solar concentrators one is dealing with unpolarized light and the choice for one of the two types of gratings will be based on the possibility to fabricate them with the desired parameters. Efficient polarization gratings cannot be realized with pitch sizes of the order of the wavelength of light using common methods and materials. Surface relief gratings on the other hand can be made with small pitch sizes and relief structures result in
high $\Delta n$-values. Furthermore, they are relatively easy to reproduce. Surface relief gratings are therefore the better choice for solar concentrators.

Here the definition of the parameter defining thick and thin was not an issue. For our application and based on the observations in this paper, it would be more convenient to define thin in a phenomenological way: a grating is thin when a value of $d$ can be achieved for which the 0th order vanishes.

In order to compare simulations with experiments, we only considered $\lambda = 633\text{nm}$, variations in polar angle $\theta$ and s-polarization. Since the physically important length scales are not the actual wavelength, pitch size and thickness, but rather their ratios, the same conclusions hold for different wavelengths by adjusting $\Lambda$ and $d$ appropriately. A surface relief grating shows hardly any polarization dependence (none in the Fraunhofer approximation) when it is really thin. Usually, the grating becomes more polarization dependent when it becomes less thin and higher diffraction efficiencies can be obtained for s-polarization than for p-polarization. Finally, conical incidence is of importance for in-coupling applications. We expect that for non-zero azimuths still surface relief gratings will be more suited than polarization gratings.

6. Conclusions

Using transmission gratings light can be coupled efficiently into a light guide for a specific, limited range of incoming angles. Liquid crystal-based polarization gratings and classical surface relief gratings have comparable diffraction efficiency and angular acceptance as long as their thickness-parameters are within the same regime. Efficient polarization gratings with small pitch sizes required for in-coupling applications cannot be realized using standard techniques and materials. For applications involving unpolarized light and/or requiring small grating periods, such as solar concentrators, surface relief gratings are preferred over polarization gratings.

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