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 a low angular and wavelength dispersion could be used to collect sunlight in a light guide. In this paper we compare the diffractive properties of polarization gratings and classical surface-relief gratings and explore their possible use in solar concentrators. It is found that polarization gratings and surface-relief gratings have qualitatively comparable diffraction characteristics when their thickness parameters are within the same regime. Relatively large grating periods result in high diffraction efficiencies over a wide range of incident angles. For small grating periods the efficiency and the angular acceptance are decreased. Surface-relief gratings are preferred over polarization gratings as in-couplers for solar concentrators.

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References and links

1. Introduction

Solar energy could be 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 it economically competitive and suitable for large-scale use, these costs have to 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, this is done with high concentration ratio systems consisting 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 low concentration ratio system can be based on a plastic light guide, resulting in an inexpensive, flat and lightweight solar concentrator. Sunlight is coupled into the light guide and then guided towards a small solar cell via total internal reflection (TIR). Producing a solar concentrator in this way requires structures that efficiently couple sunlight into a light guide (i.e. bring it into TIR). Several ways to do so have been studied and all have disadvantages. Refractive structures are bulky. Scattering elements always lead to a 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 orders. If the diffraction angle of a specific order is larger than the critical angle of the light guide material,
Fig. 1. Sketch of a grating for in-coupling applications. Here, the $+1^{st}$ order ($m = 1$) is transmitted into TIR for all angles of incidence, while the $0^{th}$ order ($m = 0$) is lost. The $-1^{st}$ order ($m = -1$) is transmitted into TIR for small angles of incidence and is lost for larger values of $\theta$.

that order will be transmitted into TIR (Fig. 1). In order to obtain such a large diffraction angle, a relatively small grating period (or pitch size) is required. For solar concentration, the grating should have a high diffraction efficiency (i.e. a low $0^{th}$ order, since this constitutes loss). In order to minimize tracking and to capture diffuse sunlight, the grating should be as insensitive to the angle of incidence as possible. Finally, for sunlight, unpolarized light and a broad spectrum of wavelengths need to be taken into account. Diffractive concentrators are subject to the constraints imposed by the brightness theorem [7, 8], which in the end restricts to what extent a system can combine high efficiency with angular and wavelength acceptance.

In this paper we study what characteristics a grating should have in order to be useful as an in-coupler for solar concentrators. 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 $0^{th}$ order and the angular dependence of the diffraction efficiency, and determine to what extent they meet the requirements for solar concentrators. From this study we determine what grating parameters 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 and optical or e-beam lithography. Although most considerations will be independent of the production technique, the gratings considered in this paper are produced holographically. Holographic production can be done relatively fast and provides easy control over grating parameters. Two coherent beams generate an interference pattern with a periodicity $\Lambda$ given by $\Lambda = \frac{\lambda_{\text{rec.}}}{2 \sin \theta_{\text{rec.}}}$, where $\lambda_{\text{rec.}}$ is the wavelength of the recording beams and $\theta_{\text{rec.}}$ the half angle separating them. This pattern is recorded in a photosensitive material. We distinguish between two forms of holography: normal intensity holography, resulting in surface-relief gratings and polarization holography (with a periodic variation of the polarization), resulting in polarization gratings.

For normal intensity holography both recording beams are s-polarized. Their interference pattern is constant in polarization, equal to the polarization of the recording beams, and fluctuates in intensity. A photosensitive material (or photoresist) records 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
3. Surface-Relief Gratings

Surface-relief gratings are interesting for large-scale applications, since they can be reproduced relatively easily from a master. Classically, isotropic gratings can be categorized as either thick or thin [14]. Thick gratings show Bragg diffraction. Their diffraction efficiency can be approximated analytically using Kogelnik’s coupled wave theory [15], 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 [16]. When a beam is diffracted by a thin grating, the Fraunhofer approximation for the (scalar) far field \( E_m \) of the \( m \)th transmitted diffraction order can be written as:

\[
E_m = \frac{1}{\Lambda} \int_{0}^{\Lambda} E_{\text{in}} \exp[-2\pi i(m x / \Lambda + d n(x) / \lambda)] \, dx, \tag{1}
\]

where \( \Lambda \) is the grating period, \( E_{\text{in}} \) the (scalar) field of the incident beam, \( \lambda \) the incident 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 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 transmitted diffraction efficiencies \( \eta_m = |E_m|^2 / |E_{\text{in}}|^2 \) are obtained. A sinusoidal profile leads to the well-known Raman-Nath expression [17]. The efficiency of the \( m \)th order is given by:

\[
\eta_m = J_m^2 (\pi \Delta nd / \lambda), \tag{2}
\]

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

\[
\eta_m = \begin{cases} 
\sin^2 \left( \frac{m \pi}{2} \right) \cos^2 \left( \frac{\pi \Delta n d / \lambda - m \pi / 2}{2} \right), & \text{for } m = 0; \\
\cos^2 \left( \frac{\pi d \Delta n / \lambda}{2} \right), & \text{for } m = 2k + 1; \\
\frac{4}{(m \pi)^2} \sin^2 \left( \frac{\pi d \Delta n / \lambda}{2} \right), & \text{for } m = 2k, \ k \neq 0,
\end{cases} \tag{3}
\]

where \( k \in \mathbb{Z} \).
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 expressions for Bragg and Raman-Nath diffraction result in reasonable approximations. This is done by comparing the grating thickness \( d \) and the wavelength \( \lambda \) with \( \Delta n \) and/or the average index of refraction \( \bar{n} \) and the grating period \( \Lambda \). Most often, the Klein parameter \([18]\),

\[
Q = \frac{2\pi d\lambda}{\bar{n}\Lambda^2},
\]

is used and a grating is considered thin when \( Q < 1 \) and thick when \( Q > 10 \). Another frequently used parameter is \([17]\):

\[
\rho = \frac{2\lambda^2}{\bar{n}\Delta n\Lambda^2},
\]

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, different parameters may be chosen for different regimes. The definition of the regimes may depend on the situation and the chosen criterion \([19, 20]\). Consequently, the distinctive parameter and the terminology can be confusing.

Despite this ambiguity, one can always assure that a grating can be considered as thin by choosing the pitch size large enough. For low values of \( d \) the diffraction efficiency is less sensitive to the wavelength and angle of incidence \([14]\) and fluctuates less upon 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:

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

where we set \( \eta_0 = 0 \) in Eq. (2) and Eq. (3). With \( d \) of this order of magnitude and for reasonable values of \( \bar{n} \) and \( \Delta n \), \( \Lambda \gg \lambda \) leads to \( Q, \rho \ll 1 \).

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) \([21]\), the Finite-Difference Time-Domain method (FDTD) \([22]\) or the Finite Element Method (FEM) \([23]\) to determine the diffraction efficiencies. For surface-relief gratings we used the commercially available software GSolver \([24]\), 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 incident wavelength: \( \Lambda = 15 \mu m \) and \( \lambda = 633 \text{ nm} \), assuring that the gratings can be considered as thin.

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, of the thickness \( d \) and to see 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 refractive index \( n_{out} = 1.6 \) and that the incident light is s-polarized. The resulting 0th and ±1st transmitted orders are plotted in Fig. 2 (solid lines), together with the corresponding Fraunhofer expressions (dashed lines). The Fraunhofer approximation is followed closely for low values of \( d \). Around \( d = 0 \) the difference is mainly due to the fact that the Fraunhofer approximation does not take reflections into account, while these are considered in the RCWA calculation (reflected orders are not plotted in Fig. 2). For higher values of \( d \) the simulated results start to deviate more from the analytical approximations.
In order to study the angular dependence of a thin surface-relief grating using 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. 2 in order to maximize the diffraction efficiency and to minimize the angular dependence: $d = 2.4 \lambda / (\pi \Delta n) = 821$ nm for the sinusoidal grating and $d = \lambda / (2 \Delta n) = 536$ nm for the rectangular grating. The resulting $0^{th}$, $\pm 1^{st}$ and $\pm 2^{nd}$ transmitted orders are plotted in Fig. 3 (these do not add up to 100% due to non-plotted reflections and higher orders). 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 $0^{th}$ order at high angles of incidence. More importantly, as the angle of incidence is increased from $\theta = 0^\circ$ the diffraction efficiency initially decreases only slowly. The $0^{th}$ order remains less than 10% for angles of incidence as high as $57^\circ$ and $47^\circ$ for the sinusoidal and the rectangular grating, respectively, which seems promising for our application.

3.1.1. Experimental

Next to these simulations, we experimentally verified the low $0^{th}$ order and the wide angular acceptance for a large-period surface-relief grating produced in SU-8. To promote adhesion of the grating to the substrate, first a thin layer of SU-8 (SU-8 2000 series, MicroChem) was spin coated on a glass substrate. After evaporating the solvent the sample was flood exposed and baked at 95$^\circ$C to obtain a 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 29 wt% solution of SU-8 at 3000 rpm for 30 seconds. After evaporation of the solvent the sample was exposed in an intensity holographic setup using an Ar$^+$-laser operated at the 351 nm UV-line with a dose of approximately 14 mJ/cm$^2$. The sample was then baked at 95$^\circ$C, developed 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 (Fig. 4), the pitch size $\Lambda$ and grating thickness $d$ were measured to be approximately 15.6$\mu$m and 0.6$\mu$m, respectively.

As a reading beam, an s-polarized 633 nm HeNe-laser was used and the diffraction efficiencies of the $0^{th}$, $\pm 1^{st}$ and $\pm 2^{nd}$ transmitted orders were measured as a function of the angle of
Fig. 3. Calculated (RCWA) transmitted diffraction efficiency as a function of the angle of incidence for a thin surface-relief grating in SU-8: \( \Lambda = 15 \, \mu m, \lambda = 633 \, nm \), s-polarization. (a) Sinusoidal surface-relief profile with \( d = 821 \, nm \). (b) Rectangular surface-relief profile with \( d = 536 \, nm \).

Fig. 4. Confocal microscopy image (a) and corresponding cross section (b) of a thin surface-relief grating in SU-8: \( \Lambda \approx 15.6 \, \mu m, d \approx 0.6 \, \mu m \).

Fig. 5. Measured (a) and calculated (RCWA) (b) transmitted diffraction efficiency as a function of the angle of incidence for an experimental thin surface-relief profile in SU-8: \( \Lambda \approx 15.6 \, \mu m, d \approx 0.6 \, \mu m, \lambda = 633 \, nm \), s-polarized light.
incidence. The results are plotted in Fig. 5(a). Next, a profile for this particular grating was derived from the confocal microscopy images (Fig. 4) and used to calculate the angular dependence for this particular experimental profile using RCWA. These RCWA results are shown in Fig. 5(b). The measured and simulated results are in good agreement. It is observed that the $0^{th}$ order indeed remains low for a wide range of incident angles. Most interestingly, the efficiencies of the $±1^{st}$ and $±2^{nd}$ orders are high and relatively insensitive to the angle of incidence. The observed behavior of the diffraction efficiencies is in between that expected for a sinusoidal and a rectangular grating (cf. Fig. 3), as to be expected, since the profile observed in Fig. 4 is neither a perfect sine, nor a perfect rectangle.

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. For the case at hand, a surface-relief grating in SU-8 with $n_{SU-8} = 1.59$ and $n_{air} = 1$, we obtain $\bar{n} = 1.295$ and $\Delta n = 0.59$. The grating period is limited by the requirement that light should be transmitted into TIR. From the grating equation it is easily seen that at normal incidence a grating period equal to the wavelength of the incident 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: $m\lambda / \Lambda = n_{out} \sin (\theta_{st})$ gives $\theta_{±1}(\Lambda = \lambda) = ± \arcsin (1/n_{out}) = ± \theta_{crit}$. In practice $\Lambda \lesssim \lambda$ is taken to obtain a small range of angles of incidence that is transmitted 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. (7) as an upper bound, one can estimate $d \lesssim \Lambda \lesssim \lambda$. Inserting these estimates into the definitions for $Q$ and $\rho$, 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 [24].

The possibility to design a grating with a vanishing $0^{th}$ 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 extent these properties still hold for surface-relief gratings with $\Lambda \lesssim \lambda$, suitable for transmitting light into TIR. This is done assuming a grating with a sinusoidal or a rectangular profile in SU-8 with a period $\Lambda = 600$ nm, applied on top of a light guide with $n_{out} = 1.6$ and for $s$-polarized light with wavelength $\lambda = 633$ nm.

First, the grating thickness $d$ is varied at normal incidence. The results are plotted in Fig. 6. 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 gratings in Fig. 2 and with a smaller periodicity.

The angular dependence of a non-thin $\Lambda = 600$ nm surface-relief grating was studied analogous to the case of the thin $\Lambda = 15$ $\mu$m grating. The thickness $d$ was chosen at the first maximum of $\eta_{±1}$ in Fig. 6: $d = 410$ nm for a sinusoidal grating and $d = 351$ nm for a rectangular grating. The results are plotted in Fig. 7. The rectangular profile performs slightly better at small angles of incidence and the sinusoidal grating has a higher $-1^{st}$ and a lower $-2^{nd}$ order at large angles of incidence. However, the differences are not as explicit as in the case of thin gratings (cf. Fig. 3) 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.

More importantly, comparing Fig. 3 and Fig. 7, we see that the diffraction efficiency of the non-thin gratings is much more sensitive to the angle of incidence. Both the $+1^{st}$ and $-1^{st}$ order drop quickly as $\theta$ is increased from $\theta = 0^\circ$, resulting in a high $0^{th}$ order. It can be concluded that insensitivity to the angle of incidence is a property of thin surface-relief gratings, and does not hold for the small-period, non-thin case.
3.2.1. Experimental

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

Again, a HeNe-laser ($\lambda = 633$ nm, 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 the flat surface of a PMMA hemisphere and brought into optical contact using an index matching liquid, assuring that the diffracted beams encounter the PMMA-air
Fig. 8. SEM images of the top view (a) and cross section (b) of a non-thin surface-relief grating in SU-8: $\Lambda \approx 0.59 \mu\text{m}, d \approx 0.4 \mu\text{m}$.

Fig. 9. Measured (a) and calculated (RCWA) (b) transmitted diffraction efficiency as a function of the angle of incidence for an experimental non-thin surface-relief grating in SU-8: $\Lambda \approx 0.59 \mu\text{m}$, $d \approx 0.4 \mu\text{m}$, $\lambda = 633$ nm, s-polarization.

interface at normal incidence. Subsequently, the transmitted diffraction efficiencies were measured for various angles of incidence. The results are plotted in Fig. 9(a). 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 using RCWA (Fig. 9(b)). The drop in $\eta_{-1}$ around $\theta = 5^\circ$ and the rise in $\eta_{-2}$ for large angles of incidence are less explicit in the measurement, but in general the measurement and the RCWA result are in good agreement. When compared to the large-period grating (cf. Fig. 5), we observe that for this small-period grating the $0^\text{th}$ order is indeed larger at $\theta = 0^\circ$ and shows an additional sharp rise when $\theta$ is increased, resulting in low in-coupling efficiencies.

3.2.2. 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 incident angles around $\theta = 0^\circ$ can be transmitted efficiently into TIR, due to the poor angular dependence of non-thin gratings and their non-vanishing $0^\text{th}$ order. According to the parameters $Q$ and $\rho$, Eq. (5) and Eq. (6), respectively, the thickness parameters of a surface-relief grating can also be decreased using a material with a higher refractive index, thus increasing $\bar{n}$ and $\Delta n$. We performed simulations assuming surface-relief gratings produced in a material with refractive index $n = 2.49$ (e.g. titanium dioxide),
Fig. 10. Calculated (RCWA) transmitted diffraction efficiency as a function of the grating thickness $d$ at normal incidence for a small-period surface-relief grating in a material with a high refractive index: $n = 2.49$, $\Lambda = 600\text{ nm}$, $\lambda = 633\text{ nm}$, s-polarization. (a) Sinusoidal surface-relief profile. (b) Rectangular surface-relief profile.

Fig. 11. Calculated (RCWA) transmitted diffraction efficiency as a function of the angle of incidence for s-polarized light for a small-period surface-relief grating in a material with a high refractive index: $n = 2.49$, $\Lambda = 600\text{ nm}$, $\lambda = 633\text{ nm}$. (a) Sinusoidal surface-relief profile with $d = 289\text{ nm}$. (b) Rectangular surface-relief profile with $d = 262\text{ nm}$.

$\Lambda = 600\text{ nm}$, $\lambda = 633\text{ nm}$ and s-polarized light. Figure 10 shows the transmitted diffraction efficiency as a function of the height $d$ at normal incidence for a sinusoidal (a) and a rectangular (b) profile. It is observed that, using this high refractive index, it is possible to choose a value for $d$ for which $\eta_0$ vanishes.

Furthermore, the angular dependence is improved, compared to surface-relief gratings produced in SU-8, as can be seen in Fig. 11. The 0th order is low for a wider range of incident 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 wide angular acceptance are a consequence of a low thickness parameter and not just a paraxial effect, as would still be possible based only on Sections 3.1 and 3.2. The gratings studied in Fig. 11 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.

4. Polarization Gratings

Liquid-crystal based polarization gratings can be made with 100% diffraction efficiency. In the paraxial approximation their diffraction efficiency is given by $[10, 25, 26]$:

$$
\eta_0 = \cos^2(\pi \Delta n d / \lambda),
$$

$$
\eta_{\pm1} = \frac{1 \mp S'_3}{2} \sin^2(\pi \Delta n d / \lambda),
$$

where $S'_3$ is the normalized Stokes parameter of the incident 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 by $d = \lambda / 2\Delta n$. Furthermore, previous simulations indicated that the diffraction efficiency of polarization gratings is relatively insensitive to the angle of incidence [11]. Based on these arguments, they seem to be a good choice as gratings for in-coupling applications.

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. Also, so far the wide angular acceptance has only been 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 experimentally verify the good angular acceptance that was found numerically by Xu et al. [11] for large-period polarization gratings and study to what extent it still holds for small periods, useful for in-coupling applications ($\Lambda \lesssim \lambda$).

There is some work done on categorizing polarization gratings as thick and thin. In Ref. [27] it is found that the parameter $\rho$, given by Eq. (6), and not the Klein parameter $Q$, given by Eq. (5), should be used for polarization gratings. There, in the study of the parameter $\rho$, $d$ is fixed at $d = \lambda / 2\Delta n$ (assuming this minimizes $\eta_0$, according to Eq. (8)), while $d$ is a variable in the Klein parameter and not fixed in its analysis. This makes it of limited use to us here, since Eq. (8) and Eq. (9) no longer necessarily hold for small $\Lambda$. 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. (5).

It is not our goal here to determine which parameter should be used to categorize polarization 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 difference 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 cannot be attributed to polarization effects. Thus, we assume that the terminology thick and 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 surface-relief gratings, for reasonable values of $d$ (same order of magnitude as $d = \lambda / 2\Delta n$) and $\bar{n}$ and $\Delta n$ (typically $\bar{n} \simeq 1.6$ and $\Delta n \simeq 0.2$) 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 al. [11]. Using FEM they verified Eq. (8) and showed that for thin polarization gratings the diffraction efficiency can be high for a broad range of incident angles. Here we verify this experimentally. In order to compare the results with the surface-relief gratings 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 (ROP 202, 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 \( n_e \approx 1.61 \) and \( n_o \approx 1.50 \) (ZLI-2222-000-EB019802 TJ-98-009, Merck), which aligned with the fluctuating direction of the LPP (see Fig. 12(a)).

As a reading beam, an s-polarized 633 nm HeNe-laser was used and the efficiencies of the 0\(^{th}\), ±1\(^{st}\) and ±2\(^{nd}\) transmitted orders were measured for various angles of incidence. The results are plotted in Fig. 13. The total efficiency does not add up to 100\%, mainly due to reflections and scattering inside the sample. Indeed, high diffraction efficiencies \( \eta_{\pm 1} \) are observed over a wide range of incident angles and \( \eta_0 \) is remarkably low everywhere. For high values of \( \theta \), \( \eta_0 \) is even less than found by Xu et al. (Ref. [11], Fig. 9(b) for this situation), which is due to the fact that we studied a larger pitch size (Ref. [11] 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. 13 therefore agrees well with numerical predictions.

![Fig. 12. Polarization microscopy images of thin polarization gratings. (a) Polarization grating made with ZLI-2222-000-EB019802 TJ-98-009 (Merck). (b) Polarization grating made with E7 (Merck). In (b) we observe a periodically recurring misalignment. The director indicated in the picture may be \( \Lambda/2 \) off.](image)

![Fig. 13. Measured diffraction efficiency as a function of the angle of incidence for an experimental thin polarization grating: \( n_e \approx 1.61, n_o \approx 1.50, \Lambda \approx 15 \mu m, d \approx 3 \mu m, \lambda = 633 \text{ nm}, \) s-polarized light.](image)
4.2. **Small-Period Polarization Gratings**

Xu et al. also studied small-period polarization gratings at normal incidence (Ref. [11], 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 $\Lambda = 678 \text{ nm}$ and $\Delta n \approx 0.2$ at $\lambda = 633 \text{ nm}$, which results in a minimum for the $0^{\text{th}}$ order of $\eta_0 \approx 0.7$ around $d \approx 875 \text{ nm}$. We used the same numerical method, FEM [23], to study the angular dependence of this polarization grating. The calculated diffraction efficiency is shown in Fig. 14(a) 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 (cf. Fig 13). A 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. 7 and Fig. 14(a) 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 ($n_{\text{SU-8}} = 1.59$) and low index ($n_{\text{air}} = 1$) regions in an SU-8 relief grating. To show that the angular dependence of polarization gratings is comparable to that of surface-relief gratings when 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: $n_c = 1.59, n_o = 1$ and $d = 323 \text{ nm}$. The resulting transmitted diffraction efficiency is plotted in Fig. 14(b), as a function of the angle of incidence. The higher birefringence results in higher diffraction efficiencies, around 30%, for the $\pm 1^{\text{st}}$ 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. 7.

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. (8) and Eq. (9) hold and a smaller $d$, to be found numerically,
when Eq. (8) and Eq. (9) no longer hold. In this section we address the question whether this thickness is practically realizable for a small-period polarization grating. To do so, one has to determine whether the nematic liquid crystal will align according to the director

\[ \mathbf{n} = (\cos \theta_n \cos \phi_n, \cos \theta_n \sin \phi_n, \sin \theta_n) = (\cos(\pi x/\Lambda), \sin(\pi x/\Lambda), 0), \]

(10)
as imposed by the LPP-alignment layers. This means that the corresponding free energy density, given by [28]

\[ F = \frac{1}{2} K_1 (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \times \nabla \times \mathbf{n})^2 \]
\[ = \frac{1}{2} \left( \frac{\pi}{\Lambda} \right)^2 [K_1 \sin^2 (\pi x/\Lambda) + K_3 \cos^2 (\pi x/\Lambda)], \]

(11)

(12)

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 \( d \). If 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. 12(b), which shows a polarization micrograph for a grating obtained using another liquid crystal (E7, Merck), some distortions in the alignment pattern arise that are not present in Fig. 12(a). An explanation could be that the free energy density \( F \), as given by Eq. (12), fluctuates more with \( x \) when the difference between \( K_3 \) and \( K_1 \) is larger (\( K_3 - K_1 \) is known to be relatively large for E7 in Fig. 12(b) [29], while it is small for the liquid crystal in Fig. 12(a)). This makes some regions energetically less favorable than others and the alignment might get distorted more easily. Intuitively, one may therefore assume that liquid crystals with large \( K_3 \) and small \( K_3 - K_1 \) result in 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. (10) does not correspond to a minimum of the total free energy when the thickness \( d \) exceeds a certain critical value \( d_c \). [29, 30]. 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. [30]. The requirement \( d \leq \Lambda/2 \) 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 \( \Delta n \) (e.g. for the grating in Fig. 14(a) \( d \geq \Lambda \) is required). Liquid-crystal based polarization gratings with \( d \approx \Lambda \lesssim \Lambda \) can therefore not be realized experimentally.

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 0th 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 (cf. Eq. (4) and Eq. (8)) and these higher orders can be very low, especially for low values of \( d \). Also the angular dependence (Fig. 3(b) and Fig. 13) is similar, especially for the \( \pm 1^u \) orders.

The changes upon going from large-period, thin gratings to small-period, non-thin gratings are comparable as well for surface-relief and polarization gratings. For common values of \( \Delta n \), it is no longer possible to obtain a vanishing 0th order and beyond normal incidence the diffraction
efficiency drops. 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. 7 and Fig. 14(b)) 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 that of surface-relief gratings. The commonly mentioned low 0th order and wide angular acceptance 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 for $d$ can be chosen for which the 0th order vanishes.

In order to compare simulations with experiments, we 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 will 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 and will be the subject of upcoming study.

6. Conclusions

Using transmission gratings, light can be coupled efficiently into a light guide for a specific, limited range of incident angles. Liquid-crystal based polarization gratings and classical surface-relief gratings have comparable diffraction efficiencies and angular acceptance as long as their thickness parameters are within the same regime. Efficient polarization gratings with small pitch sizes, as 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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