

Chirped grating IR-filter on a waveguide for sensing applications [†]

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Abstract: We present results for a specific filter design for silicon waveguides, which features transmission wavelength and bandwidth well suited for carbon dioxide sensing. Simulations were performed using Comsol Multiphysics and the design was optimized for a central wavelength of 4.26 μm . Furthermore, we included real-world effects like the discrete resolution of the design grid as well as process specific fabrication tolerances. The devised structures were based on a photonic waveguide concept, which was developed recently for evanescent-field based sensing applications. Slab waveguides with gratings on top as well as strip waveguides with sidewall gratings were considered. The concept and design are discussed in detail in order to highlight the underlying ideas.

Keywords: optical filters; silicon waveguides; waveguide filter; gratings

1. Introduction

Very recently, we proposed a novel concept for a mid-infrared bandpass filter based on a single linearly chirped Bragg grating [1]. By its design, the filter structure features a large rejection bandwidth and can be used to create narrowband emitters in the mid-infrared region. Here we present results for a specific filter design for silicon waveguides, which features transmission wavelength and bandwidth well suited for carbon dioxide sensing.

Simulations were performed using Comsol Multiphysics® and the design was optimized for a central wavelength of 4.26 μm . Furthermore, we included real-world effects like the discrete resolution of the design grid as well as process specific fabrication tolerances. The devised structures were based on a photonic waveguide concept, which was developed recently for evanescent-field based sensing applications [2]. In short, a thick SiO_2 cladding layer and an intermediate thin Si_3N_4 layer with a thickness of 140 nm are deposited on a Si substrate. The waveguide itself consists of polysilicon and it is deposited on top of the Si_3N_4 layer with a height of 660 nm. Specifically slab waveguides with gratings on top (with a modulation depth of 100 nm) were investigated.

The concept and design are discussed in detail in the following.

2. Materials and Methods

The basic structure of the filter concept is a grating with a linearly varying grating period, as sketched in **Error! Reference source not found.** Different fabrication variants are possible in order to realize actual devices featuring such a periodically varying structure. In our simulations we always considered a slab waveguide with periodical variations in structure height.

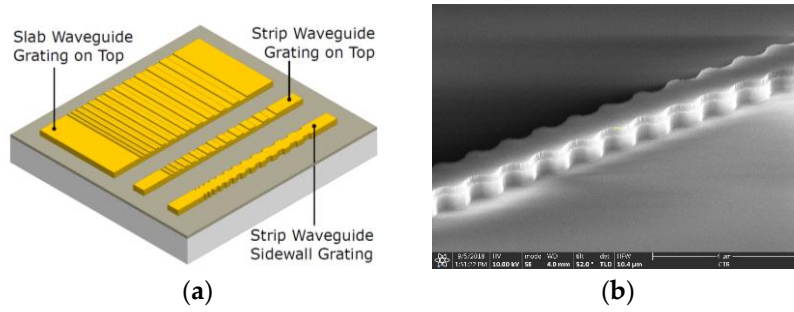


Figure 1. (a) A schematic representation of chirped gratings on slab and strip waveguides [1]. (b) SEM image of a fabricated strip waveguide with sidewall grating.

In such a grating we observe different processes depending on the ratio of grating period and wavelength. First, of course, a Bragg grating leads to a reflection in a rather narrow spectral band at a specific design wavelength. At the same time wavelengths, which are significantly smaller than the design wavelength, are diffracted out by the grating structure (This effect is used, for example, in grating coupler structures). In order to widen the reflection regime, i.e. to broaden the stop band, a chirped grating can be used, where the grating period is varied continuously over the length of the grating. This can be viewed as a sequence of Bragg gratings in series, with a systematic continuous tuning of the design wavelength. If properly designed such a grating creates a narrow transmission band in between the diffraction and the Bragg reflection regime of the grating at the spectral position of the designed transmission wavelength. The maximum wavelength which can be covered by Bragg reflection is limited due to the fact, that, if the grating pitch is further increased, also the diffraction regime is extended to longer wavelengths. Eventually this would lead to diffraction of the desired transmission wavelength. Therefore, we propose a design which utilizes a chirped grating and, at higher wavelengths, material absorption. Material absorption is used to suppress wavelengths in the sub-wavelength regime, which can be achieved by choosing materials with suitable optical properties. This allows to create a narrow transmission band with a spectrally broad reflection band by tuning the waveguide dimensions and by choosing materials with optical parameters that meet the needs of the design. In total, the filter combines three physical effects: diffraction, Bragg reflection and absorption.

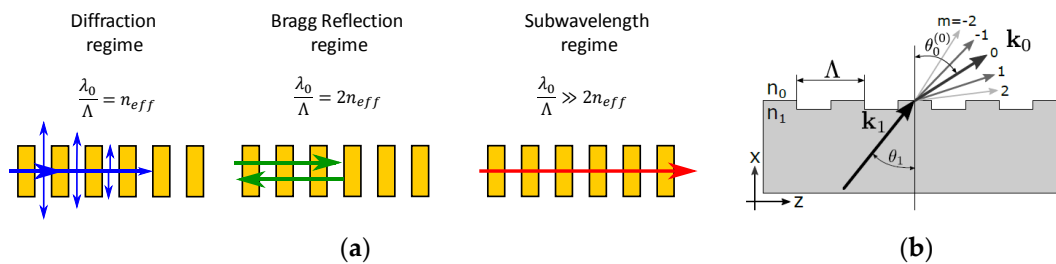


Figure 2. (a) A schematic representation of the different processes occurring for different wavelength to grating-period ratios. (b) Schematic representation of a diffraction grating on top of a waveguide, to illustrate the geometry considered in the mathematical description. [1].

Theory

Diffraction occurs if the following relation between incoming and outgoing wavevector holds

$$\beta_{in} - \beta_{scat} = \frac{2\pi m}{\Lambda}.$$

Here β_{in} and β_{scat} are the propagation constants of the modes for the incoming and the scattered wave, respectively, Λ is the pitch of the grating and m is the diffraction order.

For this work we assume a single mode propagating towards the grating region with

$$\beta_{in} = n_{eff} |k_0| = \frac{2\pi n_{eff}}{\lambda_0}.$$

n_{eff} , λ_0 , and $k_0 = \frac{2\pi}{\lambda_0}$ are the effective mode index, the vacuum wavelength and the wavevector in vacuum, respectively.

For the case of a single fundamental quasi-TE mode in the waveguide, as assumed throughout this work, different situations can be distinguished, depending on the wavelength:

(i) Bragg reflection is the case where the incoming mode is directly reflected by the grating. This corresponds to $\beta_{scat} = -\beta_{in}$ and we obtain the condition

$$2 \beta_{in} = 2 n_{eff} |k_0| = \frac{2\pi m}{\Lambda}.$$

From this we can deduce the condition for the resonance wavelength at a given grating period $\lambda_0 = \frac{2n_{eff}\Lambda}{m}$ or similarly the condition for the grating period, corresponding to a given design wavelength $\Lambda = \frac{m \lambda_0}{2n_{eff}}$.

(ii) More generally we can expect reflection into waveguide modes for the conditions $\beta_{in} + \beta_{scat} = \frac{2\pi m}{\Lambda}$ which leads to the condition $\Lambda = \frac{m \lambda_0}{n_{in}^{eff} + n_{scat}^{eff}}$. Since the lowest order mode has the highest effective index of refraction we can expect, that scattering towards backpropagating higher order modes happens at a smaller ratio of $\frac{\lambda_0}{\Lambda}$ (c.f. **Error! Reference source not found.**(a)). Thus, for a given grating period it will happen at smaller wavelengths, as already outlined above.

(iii) The second regime is diffraction out of the waveguide into the radiative modes. These modes form a continuum. The resonance condition is best described in terms of the scattering angles θ_1 . (see **Error! Reference source not found.**(b); note that $n_{eff} = n_1 \sin(\theta_1)$.) The grating equation can be formulated

$$n_1 \sin(\theta_1) - n_0 \sin(\theta_0^m) = \frac{m \lambda_0}{\Lambda}.$$

Thus the angle at which a given wavelength is diffracted out of the waveguide is given by the relation: $\sin(\theta_0^m) = \frac{1}{n_0} \left(n_{eff} - \frac{m \lambda_0}{\Lambda} \right)$. Scattering perpendicularly away from the waveguide corresponds to $\theta_0^m = 0$ and happens for the condition that $\frac{m \lambda_0}{\Lambda} = n_{eff}$. The whole regime of scattering occurs for $\frac{m \lambda_0}{\Lambda} = n_{eff} - n_0$ to $\frac{m \lambda_0}{\Lambda} = n_{eff} + n_0$.

Generally, for a given grating period diffraction happens at shorter wavelengths than Bragg reflection. And between the diffraction regime and the reflection there is a specific gap, where light is transmitted through the waveguide without perturbation.

When focusing on the lowest order of diffraction ($m=1$) this gap extends from $\frac{\lambda_0}{\Lambda} = n_{eff} + n_0$ to $\frac{\lambda_0}{\Lambda} = 2n_{eff}$. We see, that already a simple Bragg grating provides not only a sharp reflection band, but also contains introduces blocking due to scattering at lower wavelength and in between features a band with high transmission with a bandwidth of $\Delta\lambda_0 = \Lambda(n_{eff} - n_0)$.

Design and Modelling

Our model is based on recent investigations towards an integrated evanescent field NDIR sensor platform. The waveguide is formed by a 660 nm poly-Si layer, which is placed on a thin Si₃N₄ substrate, which also acts as an absorbing layer. Below we have a thick SiO₂ layer, on a Si substrate, which prevents leaking of the mode to the substrate. On the waveguide a grating is formed with a depth of 100 nm and a pitch, which is typically linearly increasing.

The simulations were done using COMSOL Multiphysics 5.4. A detailed description of the model can be found in [1].

For the modeling, we considered the SiO₂ layer below the waveguide to be infinitely extended. On both sides of the grating the unperturbed waveguide was elongated. In these sections numerical ports (Num. Port), and an evaluation boundary (Eval. Bound.) were placed. Furthermore, the simulation domain (total thickness 5 μm) was terminated on all sides by perfectly matched layers (PML) and scattering boundary conditions (SBC) in order to absorb radiation that reaches the domain boundary in order to avoid interference with spurious reflections. On the left side, two numerical interior ports were used, one to excite and detect the fundamental quasi-TE mode and the other one

to account for reflections of the first higher order quasi-TE mode. On the right-hand side both numerical interior ports were used to analyze the transmitted radiation of the two lowest order quasi-TE modes. These interior ports do not absorb radiation and do not affect the wave pattern passing by. In order to determine the total reflection and transmission, the normal power flow through the evaluation boundary on both sides of the grating is evaluated.

The chirped grating geometry was created using a Java code in the COMSOL application builder. The center pitch was 753 nm (calculated using Equation (3.6)), with the mean effective mode index for elevations and wells. The grating pitch was increased up to a maximum pitch of 1011 nm. On both ends of the filter, the waveguide was extended by 8 μm beyond the grating region, including the port, evaluation boundary and a 1 μm PML section. Three configurations for the grating pitch repetitions ($N = 1, 4, 8$) were investigated, leading to grating lengths of 106.8 nm, 427.2 nm and 854.4 nm respectively.

Within this work literature values were used for the materials (Air [3], Si [4], Si_3N_4 [5], SiO_2 [5]), which can be easily accessed and are already implemented in COMSOL.

3. Results and Discussion

For a better understanding we start the discussion with a simple grating featuring a constant pitch. **Error! Reference source not found.** shows simulation results on a grating with 480 lines and a pitch of 771 nm. The pitch was chosen with a passband of 4.26 μm in mind, meaning that the reflection is designed to occur slightly detuned on the long wavelength side. **Error! Reference source not found.**(a) displays the reflectivity of the grating, i.e. the relative intensity of the mode reflected back by the grating within the waveguide. In fact, there are two bands. The Bragg reflection, reflecting the TE_0 mode back, has a maximum at 4.35 μm . The second peak at about 3.5 μm corresponds to back scattering into the TE_1 mode. This can also be discerned in **Error! Reference source not found.**, where the electric field distribution at the grating is displayed. At 4.35 μm and at 3.5 μm the whole incoming mode is reflected at the beginning of the grating and there is no significant energy left behind the grating. And while, at 4.35 μm we see the symmetric TE_0 mode, at 3.5 μm , there is a clear anti-symmetric shape reflecting the symmetry of the back-reflected TE_1 mode, which transports nearly all the energy in this case.

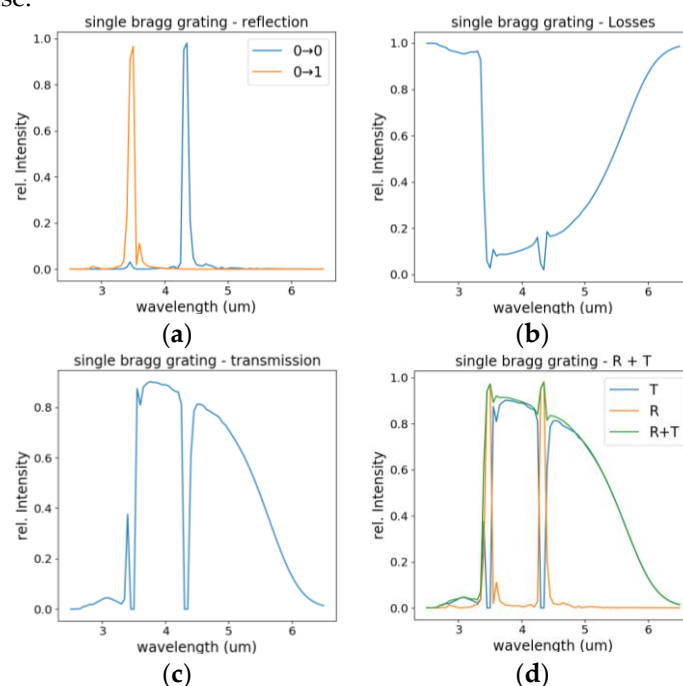


Figure 3. Simulation results for a Bragg grating with 480 lines and a pitch of $\Lambda = 0.771 \mu\text{m}$.

If we look at the total losses from the waveguide (**Error! Reference source not found.**(b)), meaning the energy which is lost from the waveguide, we see a strong contribution on the short

wavelength side up to about 3.4 μm . This corresponds to the scattering regime, where the energy is scattered out. In the following regime (above 3.4 μm) the energy is kept within the waveguide (reflected or transmitted) but with increasing damping due to absorption (see **Error! Reference source not found.**(b)). The absorption is mainly caused by the Si_3N_4 -layer with also some contributions from the SiO_2 . Both materials feature some absorption in the MWIR regime, which becomes significant for longer wavelengths. **Error! Reference source not found.**(c) shows the transmission through the waveguide, where the losses from the waveguide as well as the blocking due to reflection show up. Finally, **Error! Reference source not found.**(d) shows reflection and transmission on the same graph.

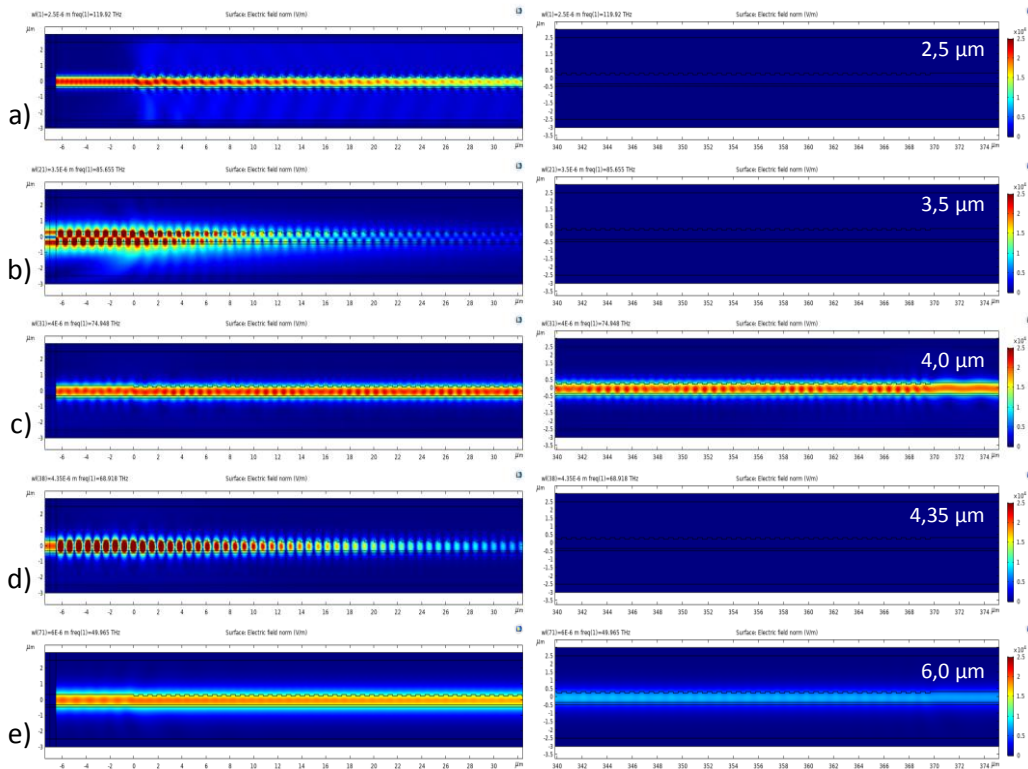


Figure 4. Plots of the electric field at the Bragg grating for selected wavelengths. Grating parameters were identical to those of **Error! Reference source not found.**. Plotted is the amplitude of the electric field at the beginning (plot on the left-hand side) and at the end of the grating (plot on the right-hand side) for initial excitation with a TE_0 mode from the left. The wavelengths are (a) 2.5 μm , (b) 3.5 μm , (c) 4.0 μm , (d) 4.35 μm , and (e) 6.0 μm .

Error! Reference source not found. shows the effective refractive indices of the first three waveguide modes. These are the two lowest-order TE-modes as well as the fundamental quasi-TM mode. The latter was not considered at all in the simulations, since, if the initial state is the quasi-fundamental TE mode, mixing to quasi-TM modes does not play a significant role. **Error! Reference source not found.**(a) shows the real part n_{eff} and **Error! Reference source not found.**(b) the imaginary part k of the mode indices. The imaginary part is responsible for damping and we deduce, that for longer wavelengths damping within the waveguide provides significant blocking, which is important for the functionality of the broad band filter.

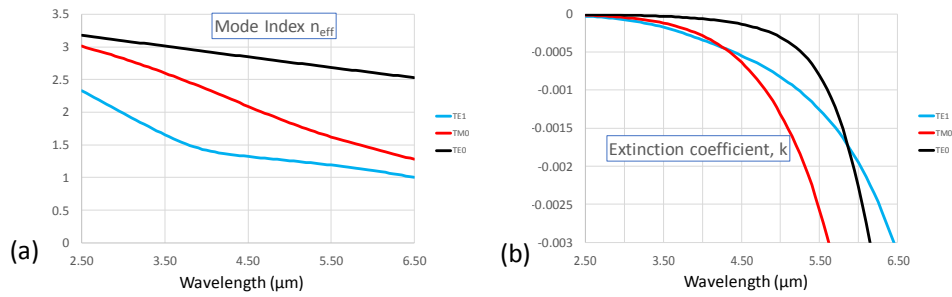


Figure 5. (a) Real part and (b) imaginary part of effective refractive indices of the three lowest order modes, which are the two lowest-order TE-modes as well as the fundamental quasi-TM mode.

The transmission curve of a single Bragg grating (**Error! Reference source not found.**(c)) already defines a filter curve, albeit not an adequate one, with regard to the goal of developing a narrow band transmission filter. However, one could imagine, to combine a series of such gratings, all with different grating constants, in order to “tailor” the final transmission curve to the design goals. The idea behind the chirped grating approach is to use the combined effect of blocking by diffraction and by reflection from a grating which features a continuously varying grating constant. This is presented in much detail in **Error! Reference source not found.**, where results for Bragg grating with increasing numbers of subunits with different grating periods Λ are displayed.

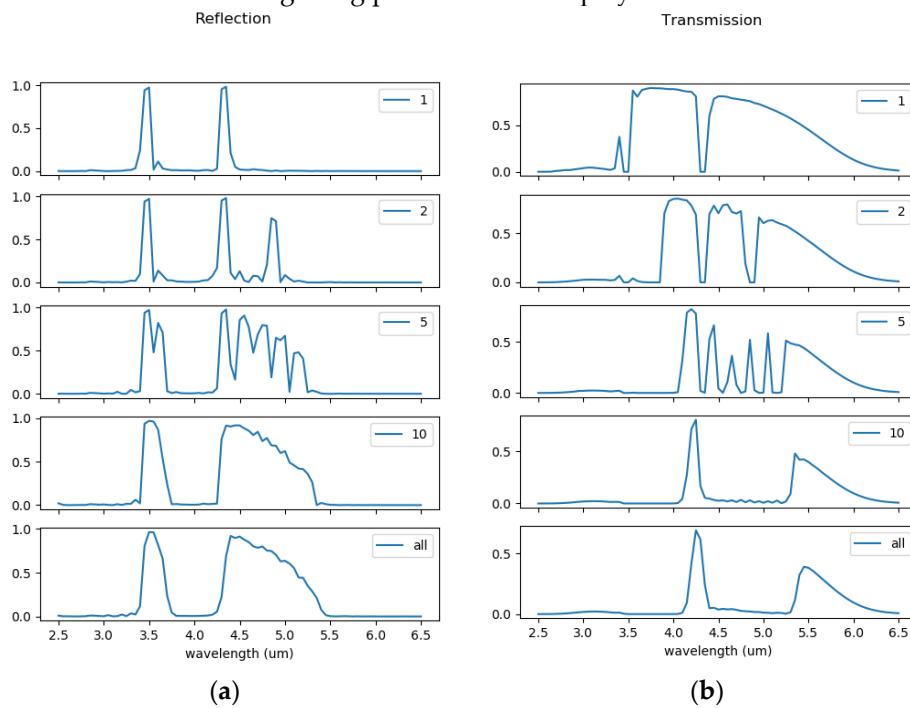


Figure 6. (a) Reflection and (b) Transmission of Bragg grating with increasing number of subunits with different grating periods Λ as indicated in the legends. In each case the overall grating had 480 lines. From top to bottom the number of distinct grating periods is $n_\Lambda = 1, 2, 5, 10, 480$.

In each case the overall grating has 480 lines. The upper-most row corresponds to a single Bragg grating with a period of 771 nm. Below the results are displayed for a grating with 240 lines with a grating period of 771 nm directly followed by 240 lines with a grating period of 891 nm. The bottom line then corresponds to a grating with 480 lines, where the period is continuously varied from 771 nm to 1.011 μm .

As more and more different grating periods are included in the grating, we see how the Bragg-reflection bands add together. At the same time, we see a broadening of the bands, since each contributing “sub-grating” effectively has a smaller number of lines. Already with a combination of 10 periods, a continuous rejection band is obtained, with a relatively narrow transmission band at the

target wavelength of 4.26 μm , together with some long-wavelength contribution. Changes in the transmission spectrum between the “discrete” 10-subunits grating to the continuously varying chirped grating are only minor. Note that the blocking for wavelengths above 4.26 μm directly reflects the combination of the (Bragg-)reflection bands, while in the short wavelength region it is mainly determined by the scattering processes, which dissipate the energy away from the waveguide. The reflection band at around 3.5 μm , which corresponds to scattering from the TE_0 to the TE_1 mode, lies in the same spectral region, but cannot, for itself, explain the transmission spectrum obtained.

We expect difference for chirped gratings with rising or falling chirp of the grating period. This is compared in **Error! Reference source not found.**. In particular, the reflection to the higher order ode at short wavelengths only can occur, if it happens at the beginning of the grating, because otherwise, the short wavelengths are already scattered out of the waveguide before reflection can take place. Furthermore, the intrinsic damping, which happens a longer wavelengths, is more pronounced if reflection happens at a later stage in the grating. Thus, for a grating with linearly decreasing pitch, reflection contributions are increased for longer wavelengths. The direction of the grating, however, does not play any significant role for the final transmission achieved, because for the final transmission spectrum it does not matter, if the energy is blocked by reflection or absorption or by scattering out of the waveguide.

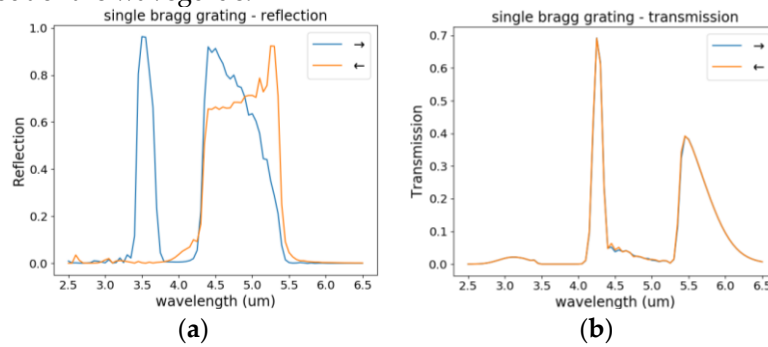
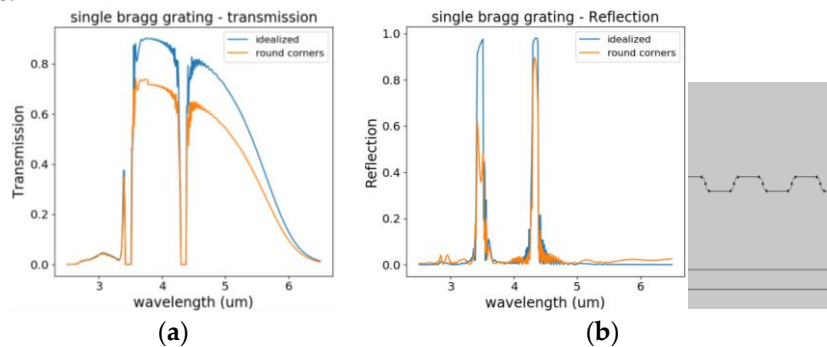


Figure 7. Comparison of the calculated (a) reflection and (b) transmission through a chirped grating when excited from the low grating-pitch side or from the high-grating pitch side. Note significant differences in the spectrum of the reflected energy, while the transmission remains nearly identical.

Real fabrication processes lead to significant rounding of the corners (An example for a strip waveguide with side-wall grating is shown in **Error! Reference source not found.**(b).) To simulate the effect from smoothing we applied a radius of 50 nm to the sharp edges of the grating (see insets of Figure 1). Simulations were performed with higher spectral resolution (wavelength steps of 5 nm), in order to more clearly distinguish the effects. The results are shown in Figure 1. Generally, the contrast which can be achieved decreases significantly, even for this minor modification. The blocking contrast does not reach 100% anymore. Otherwise the transmission curves stay very similar. This indicates, that the concept of a transmission filter based on a single chirped grating provides a robust design scheme.



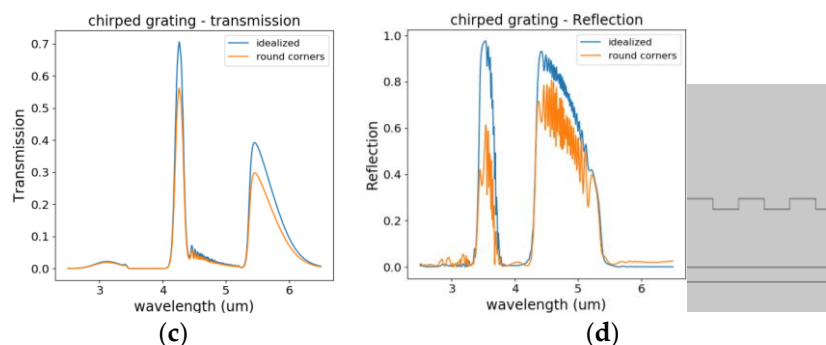


Figure 1. Comparison of a grating with idealized sharp edges to the case of round corners, with a radius of 50 nm applied. (a) reflection and (b) transmission through a single Bragg grating. (c) reflection and (d) transmission through a chirped grating with 480 lines.

4. Conclusions

In this work we proposed and investigated in much detail the concept of a linearly chirped Bragg grating for the use as bandpass filter in the mid-infrared range. To demonstrate the approach, we specifically targeted a bandpass at a wavelength of 4.26 μm , which is of high relevance for CO₂ gas sensing. Supported by simulations of simple model structures, we discussed in much detail the underlying concept and then validated the concept with realistic simulations, based on a waveguide design, which is currently used for the development of CMOS-compatible evanescent field gas sensors. In principle the presented filter can be adapted to various applications by engineering the interaction of the design and the used materials.

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Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

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