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Numerical Investigations of Infrared Slot Waveguides for Gas Sensing †

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Abstract: Sensing of gases is a promising area for applications of photonic sensor devices that operate in the mid-infrared spectral range. We present a numerical investigation of slot waveguides for evanescent field sensing of CO_2. The sensor platform is a poly-silicon slot waveguide on silicon dioxide, where both layers are deposited on a standard silicon substrate. The evanescent field ratio, which is a crucial parameter for the sensing performance of the waveguides, was determined and values as high as 42% were obtained.

Keywords: silicon photonics; mid-infrared sensing; slot waveguide

1. Introduction

In this work we present a numerical investigation of slot waveguides for evanescent field infrared absorption sensing of CO_2. Slot waveguides were first theoretically described in [1], and experimentally demonstrated in [2]. Slot waveguides offer the advantage of an increased electric field in the slot that leads to a high evanescent field ratio, which is specifically beneficial for gas sensing applications. If CO_2 is present in the slot, the evanescent field is partially absorbed by the gas, which is detected in terms of an associated damping of the guided wave. In [3], a numerical investigation of slot waveguides for CO_2 sensing using a silicon on sapphire platform was presented and an evanescent field ratio as high as ~25% was reported.

Our approach is to use SiO_2 and Si_3N_4 as materials for the lower cladding region of the waveguide. Recently we experimentally demonstrated silicon strip waveguides for CO_2 sensing using two different platforms, i.e., silicon strip waveguides on a Si3N4 membrane [4] and on a solid (Si_3N_4)/SiO_2 substructure [5]. In order to further improve the sensing performance of the waveguide structure, we aim to develop Si slot waveguides on SiO_2 with a significantly higher evanescent field ratio compared to the strip waveguides that were used in our previous work.

Figure 1 shows a schematic representation of the slot waveguide (a) and a representative field distribution of a quasi-TE mode (b), showing strong confinement of the electric field in the slot. The investigated sensor structures are compatible to fabrication on SOI wafers or on standard silicon substrates using deposited SiO_2 as substructure materials and deposited poly-silicon as waveguide material. Our ultimate goal is to develop a micro-sensor fully integrated on standard silicon substrates. Therefore, the waveguides were optimized using material parameters that were measured on deposited thin films of poly-Si and SiO_2. The waveguides were optimized for a wavelength of λ = 4.26 µm, which is at the center of the mid-infrared absorption band of CO_2 and for a gap size of 300 nm, which is compatible withstandard micro fabrication processes.

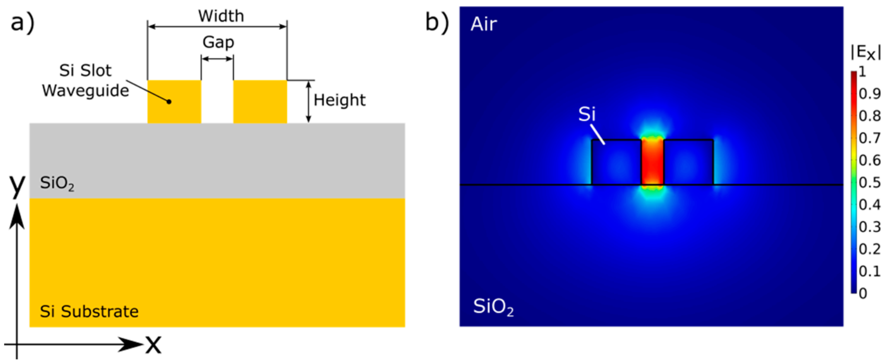

Figure 1. (**a**) Scheme of the slot waveguide (**b**) Simulation result depicting the field distribution of |Ex| for the quasi-TE mode. The results show the strong confinement of the mode in the slot.

2. Method

The FEM simulations were conducted using COMSOL Multiphysics 5.3a including the Wave Optics Module. The slot waveguides were investigated using full-vectorial FEM simulations. The domain size was 10 µm in x and y direction and was enclosed by perfectly matched layers and scattering boundary conditions in order minimize spurious reflections at the boundaries. So called "Numerical Ports" were applied on both ends of the waveguide which allow to calculate, excite and absorb specific modes. The cross-section of model was meshed with triangular elements with a maximum size of $\lambda/(8*n)$, where λ is the wavelength and n the refractive index of the individual material. Along the propagation direction the mesh of the cross-section was swept with a maximum element size of $\lambda/(8*n_{Si})$. The required optical parameters (i.e., the complex refractive index) of the used materials (SiO_2 and poly-Si) were measured on thin films prepared by low pressure chemical vapor deposition. The optical parameters were measured using a J.A. Woollam IR VASE ellipsometer.

3. Results and Discussion

The real part of the measured refractive index for poly-Si and SiO_2 is plotted in Figure 2. While the experimental results were in very good agreement with literature for SiO_2 [6], poly-Si had a higher refractive index than previously reported for bulk silicon [7]. As described, the waveguides were designed for a wavelength of 4.26 µm. The measured real part of the refractive indices at this wavelength are $n_{Si} = 3.60$ and $n_{SiO2} = 1.38$. The imaginary part (also known as extinction coefficient) at this wavelength is virtually zero for silicon and was at the noise level of the ellipsometry measurement of SiO_2. Therefore, the extinction coefficients were not considered, meaning that losses caused by absorption in the material were not considered in the simulation.

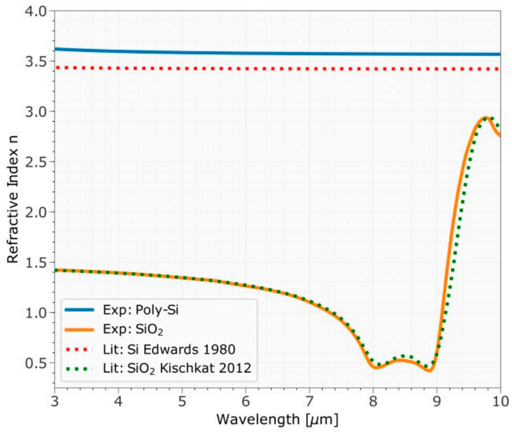

Figure 2. Experimental characterization of the real part of the refractive index n of the used materials in the mid-infrared region compared to literature values [6,7].

A 3D model of the slot waveguide was developed using COMSOL Multiphysics. The effective mode indices of the fundamental quasi-TE mode were determined conducting a modal analysis on the cross-section of the waveguide (see Figure 3a), searching for the two lowest order modes of the waveguide (modes with the highest effective mode indices). The waveguides were investigated for a gap width of 300 nm. It was found that for geometries with high aspect ratios (height/width) the fundamental mode of the waveguide is the quasi-TM mode, i.e., the mode with the highest effective mode index (not plotted). Furthermore, modes for some geometries with small waveguide widths do not fulfill the condition for guided modes ($n_{waveguide} > n_{eff} > n_{cladding}$) [8]. These modes, i.e., modes with an effective index smaller than the refractive index of SiO_2, will leak out and do not propagate over wide ranges in the slot waveguide. Figure 3c '1' shows a field distribution of such a mode. It is visible that a significant part of the mode is present in the SiO_2. The evanescent field ratio (EFR), which is a crucial parameter for the sensing application, was determined using the following equation [3]

$$EFR = \frac{\iint_{Gas} \vec{S} \cdot \vec{n}\ dxdy}{\iint_{All} \vec{S} \cdot \vec{n}\ dxdy}, \quad (1)$$

where the surface integrals extend over (parts of) the cross-sectional *xy*-plane of the waveguide, $\vec{S}$ denotes the Poynting vector and $\vec{n}$ the unit normal vector pointing in the direction of propagation.

The results are shown in Figure 3b. The highest EFR among the tested configurations was 42% for a waveguide height of 800 nm and a width of 1500 nm (see also the field distribution plotted in Figure 3c '2'). If the width of the waveguide is further increased, the fraction of the mode that is confined in the silicon part increases, which decreases the EFR of the mode (see Figure 3b and also Figure 3c '3'). As indicated in Figure 3b, choosing a higher aspect ratio leads to a higher EFR. Nevertheless, a high aspect ratio also favors the propagation of quasi-TM modes. Already for a Si height of 900 nm, the fundamental quasi-TE mode is no longer among two lowest order modes (not plotted).

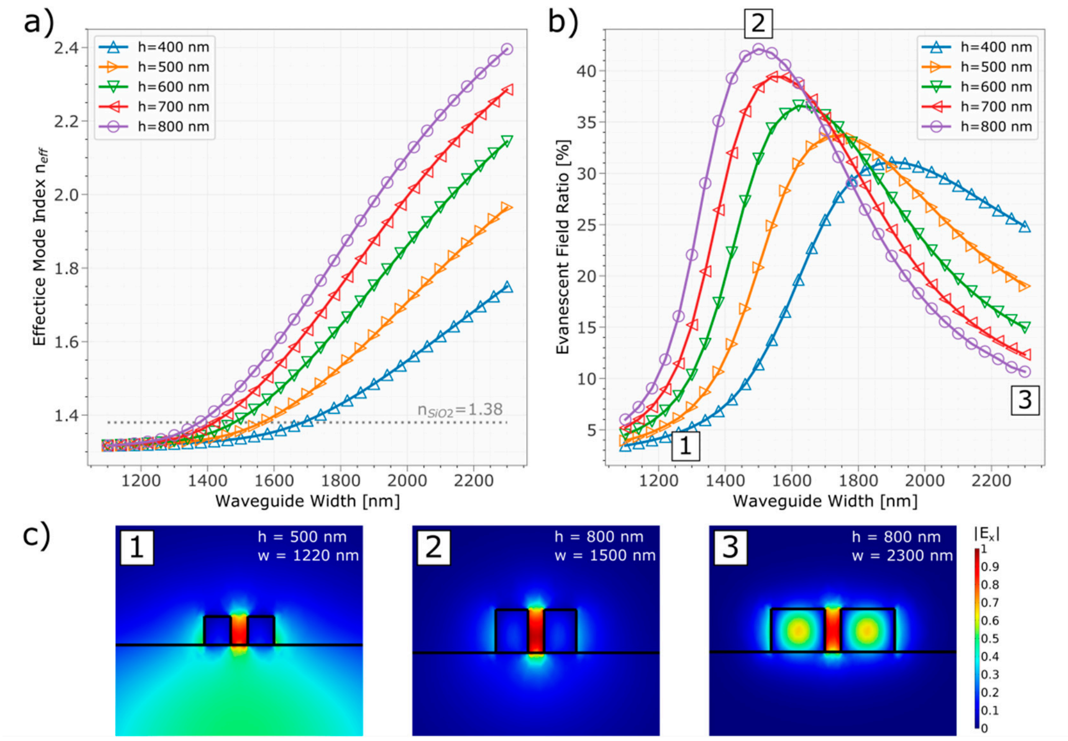

Figure 3. (**a**) Effective mode index of the fundamental quasi-TE. Modes with effective indices smaller than the effective index of SiO_2 (dotted line) are considered unguided. (**b**) The evanescent field ratio of the investigated waveguides dimensions, depicting the dominant coordinate |Ex| for the quasi-TE mode. The highest EFR was observed for a height of 800 nm and a width of 1500 nm. (**c**) Field distributions of |Ex| for some modes.

4. Conclusions

A numerical study on slot waveguides for gas sensing, using a Si on SiO_2 platform, was presented. The evanescent field ratio, which is a crucial parameter for the application of waveguides as absorption sensor, was determined. The highest evanescent field ratio that was obtained was 42%. In conclusion, this study indicates that silicon slot waveguides on a SiO_2 are promising candidates for integrated evanescent field gas sensors.

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

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