Evanescent Field Sensors Based on Si Photonics

Concept and Characterization

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***Abstract*— We present a detailed study of Si-based optical waveguides, which can be used as evanescent field sensors for the quantitative analysis of various gases and liquids. Waveguides were fabricated and experimentally characterized. Direct quantitative comparison of simulation with experimental results of directional coupling structures allows fine-tuning of the optical material parameters and provides important input for future sensor design. The concept was validated with quantitative CO_2 measurements.**

***Keywords** - silicon photonics; evanescent field sensor; directional coupler; integrated sensor.*

I. INTRODUCTION

Interest for integrated gas sensors, which could be used in mobile devices has grown over the last years and provides the motivation for investigating Si-based photonics in the mid-infrared spectral range [1]. One approach uses waveguide structures and evanescent field infrared absorption as the sensor principle [2]. The measurement principle is shown in Figure 1. Mid-Infrared radiation from a quantum cascade laser is guided to the structure via an optical fiber. Diffraction gratings and taper structures on both ends of the waveguide are used for coupling the light into and out of the waveguide. Part of the waveguide is in contact with the sample-gas and there absorption occurs in the evanescent field of the transmitted mode.

The devised active structures are silicon strip waveguides, which are in contact with the gas, so that the evanescent field gets absorbed. For a good understanding and further optimization of the sensor performance, a thorough characterization of these photonic structures is crucial. Here, we present results from simulation and experiments, where we characterized damping, mode profiles, and coupling. Comparison of simulation and experimental results also allows a fine-tuning of the simulation parameters, which is important for further optimization. Finally, our first measurements with CO_2 demonstrate the feasibility of gas measurements with this type of evanescent field sensors.

The rest of this paper is organized as follows. Section II describes experimental procedures and the fabrication of the structures. Section III presents and discusses the first results we obtained and Section IV summarizes our work and presents first conclusions from this work in progress.

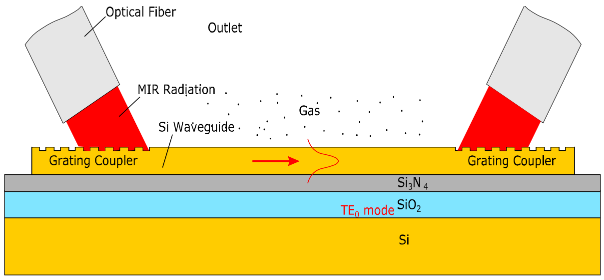

Figure 1. Schematic representation of the measurement idea. (see text for details)

II. EXPERIMENTAL

The devised sensor test structures are silicon strip waveguides on a silicon nitride-layer, deposited on SiO_2, which can be fabricated with standard semiconductor processes to provide a fully integrated CMOS (Complementary metal-oxide-semiconductor) compatible sensor.

Simulations where carried out using COMSOL-Multiphysics in order to determine favorable dimensions of the waveguide and the grating coupler. The waveguides were

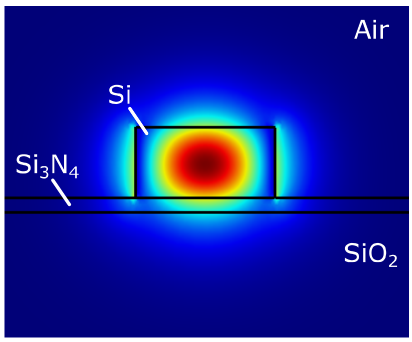

Figure 2. Field distribution of the electromagnetic field in the strip waveguide for the fundamental quasi-TE mode (a) and quasi-TM mode (b). The plot shows results for the configuration with 140 nm Si_3N_4.

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designed for the absorption band of CO_2 at 4.26 µm. The dimensions of the waveguide were chosen for single-mode wave propagation. The calculated mode profiles for a strip waveguide on a silicon nitride membrane are shown in Figure 2. The influence of different Si_3N_4 layer thicknesses on damping and mode profiles was investigated. The width and height of the waveguides are 1.4 µm and 660 nm, respectively.

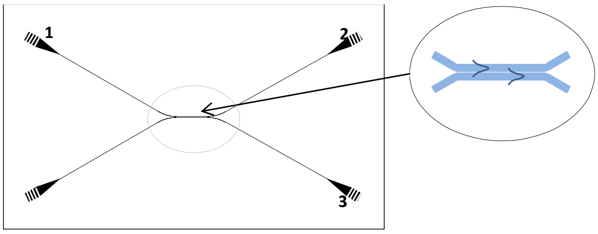


Figure 3. Scheme of the directional coupler structure. The inset on the right shows the details of the coupling region..

There are large uncertainties, with regard to the optical parameters, because the optical properties of the thin layers of poly-Si and Si_3N_4 strongly depend on the details of the deposition method. For experimental characterization of the mode properties, directional couplers were designed and fabricated, which are very sensitive to the exact shape of the mode. A direct comparison between experiments and simulation allows fine-tuning the optical parameters for the simulation. The basic outline of these structures is shown in Figure 3. A grating launch-pad with a subsequent taper structure is used to couple light in and out. Light is coupled in at port 1 and detectors are placed at port 2 ("through-port") and 3 ("drop-port"). For the structures measured in this paper, the gap between the waveguides was 400nm.

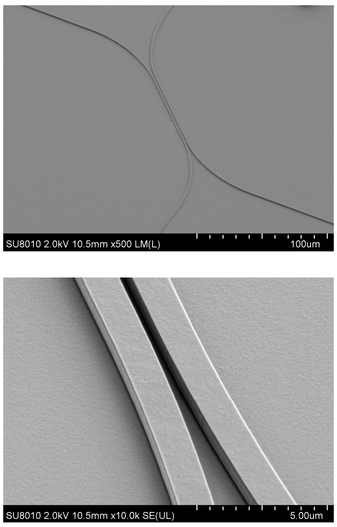


Figure 4. SEM analysis of the strip waveguide directional coupler.

Measurements on structures with different interaction lengths allow quantitative comparison of the experimental results with the simulation.

Details of the fabrication process can be found in [3]. In short, the structures were manufactured using low pressure chemical vapor deposition, lithography and etching. A 2 µm thick SiO_x layer and subsequently a Si_3N_4 layer of some nanometers were deposited onto a silicon substrate. On top of the Si_3N_4 an amorphous silicon layer was deposited which was annealed at 700 C° to achieve a polycrystalline silicon layer. Finally, the waveguide structures, as well as the gratings, where etched into the polycrystalline silicon layer.

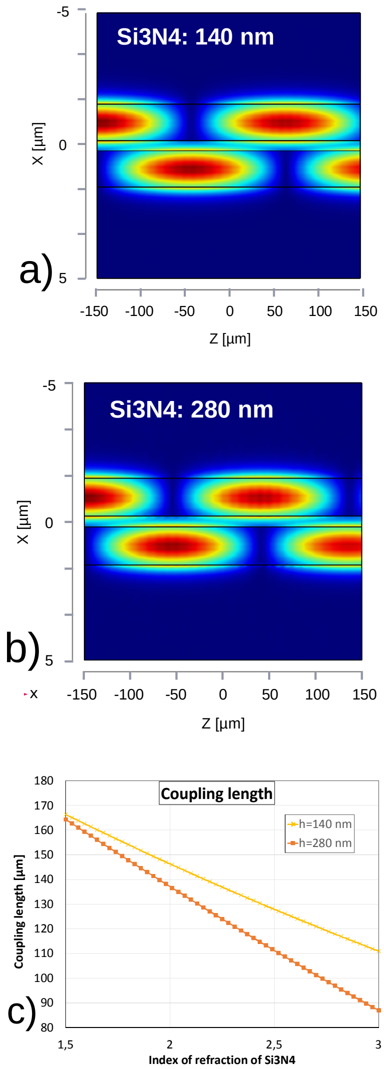


Figure 5. (a), (b) Representative simulation results for directional coupler structures with a Si_3N_4 layer thickness as indicated. The amplitude of the electric field is plotted. Optical parameters were taken from the COMSOL database. (c) Dependence of the coupling length on the index of refraction of Si_3N_4, used in the simulations.

The waveguide characterization, as well as the gas measurements, was carried out using a custom test-bench, described in detail in [4]. In short, it comprises a Quantum Cascade Laser (QCL) as radiation source, optical fibers, a stage for placing the test chips, and mercury cadmium telluride (MCT) detectors. The beam was guided from the laser to the device and from the device to the detector via optical fibers with core diameters of 100 µm and 450µm, respectively.

While the characterization of the intrinsic losses was carried out on wafer-level, the gas measurements were carried out on single chips. The single test chips were placed in a 3D printed gas cell, which comprised a gas inlet and a holder for the test chip. The top of the cell provided openings for the optical fibers, which also served as outlet for the gas. During the gas measurements the cell was flushed with CO_2/N_2 mixtures at a total flow rate of 100 ml/min using two mass flow controllers.

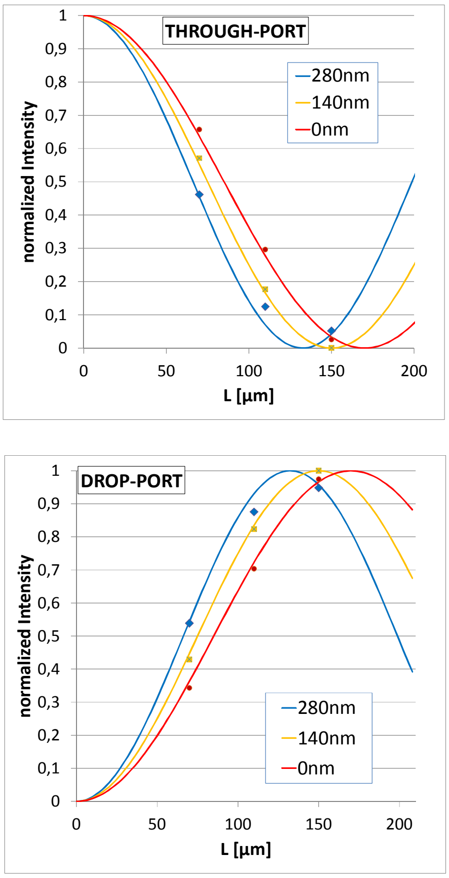
All characterization measurements were performed at 2400 cm^{-1}, which is just outside the CO_2 absorption band in order to avoid an influence of the ambient CO_2 concentration. For the absorption measurements, the laser was tuned to a position within the CO_2 band at about 2363 cm^{-1}, where maximal absorption was observed.

III. Results

Figure 4 shows pictures from scanning electron microscopy validating the fabrication quality. The surface roughness of the Si structures and the Si3N4 layer, as well as the topography of the strip waveguides were also investigated using atomic force microscopy, which revealed that the surface roughness is about 1 nm at measurement positions (on the top of the Si layer as well as on the SiO2 and the Si3N4 layer).

To measure the intrinsic losses, the transmitted IR radiation was measured on four waveguides with different lengths (5.0 mm, 7.5 mm, 10.0 mm and 12.5 mm), for each configuration of Si3N4 layer thickness (0nm, 140nm and 280nm). For every thickness, the transmitted intensity through the four waveguides was recorded, which allows to calculate the intrinsic damping, without contributions from losses at the coupling structures and the taper [5]. The damping increases with increasing Si_3N_4 thickness and is on the order of 4-5 dB/cm.

Most importantly, we performed measurements on directional couplers. These results are very sensitive to the exact shape of the mode and allow a direct comparison between experiments and simulation. Besides academic interest, this is important because it allows fine-tuning of the optical parameters for the simulation, and, in addition, such coupling structures will be important building blocks for more complex sensor designs. Figures 5(a) and 5(b) show the simulation results for two different thicknesses of the Si_3N_4 layer. From this, we estimated the coupling length for maximal energy transfer between the waveguides to be 110µm and 95µm for thicknesses of the Si_3N_4-layer of 140 nm and 280 nm, respectively. Figure 5(c) shows the calculated dependence of the coupling length as a function of layer thickness. Based on these simulations, test-structures with interaction lengths of 70, 110, and 150 µm were designed and fabricated. In the experiments, we found a mismatch of about 20% with regard to the initial estimates. However, fine-tuning of the optical parameters by some percent provides excellent overlap between experiment and simulation. This is shown in Figure 6. Here, the curves show the simulated relative intensities at the through-port and the drop-port as a function of propagation length for three different layer-thicknesses of Si_3N_4. The markers show the experimental results measured on structures with interaction lengths of 70, 110, and 150 µm and different thickness of the Si_3N_4 layer. The values for the refractive indices of Si and Si_3N_4 used in the simulations were n_{Si}=3.525 and n_{Si3N4}=1.92 respectively.



(a)

(b)

Figure 6. Comparison of simulation with experimental results. The curves show the simulated relative intensities at (a) the through-port and (b) the drop-port for three different layer-thicknesses.

Finally, in order to test the sensing capability of the strip waveguide, quantitative CO_2 measurements were conducted using a strip waveguide in the form of a meander with a length of 2 cm. The QCL was tuned to a wavelength where we observed maximal CO_2 absorption. The position of the fibers for in- and out-coupling was adjusted in order to optimize the coupling and achieve a high signal at the detector. The sensor chip was placed in a gas cell, which was flushed using mixtures of N_2/CO_2 of different concentrations. Free-beam absorption, which occurs between the fibers and

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the waveguide was characterized with a reference measurement and compensated for. In these measurements [5], it was possible to sense CO_2 concentrations down to 500 ppm, which is already in the range of the typical workplace CO_2 concentrations and well below the exposure limits.

IV. Conclusions

We presented a detailed design and characterization of silicon strip waveguides. Among others, our results indicate that the index of refraction of the deposited poly-silicon is about 3% higher in our structures, compared to literature values of bulk silicon. The waveguides feature damping characteristics of 4-5 dB/cm, depending on the details of the layer structure and can be used for CO2 monitoring, which was demonstrated with actual measurements. Based on these results, we will proceed in designing and optimizing the next generation of waveguide structures for evanescent field sensing.

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