Si Nanostrip Optical Waveguide for Molecular Overtone Spectroscopy

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Abstract

The ability to probe the molecular fundamental or overtone vibrations is central to modern health-care monitoring techniques because it provides an information about the molecular structure. However, since the absorption cross-section of molecular vibrations overtones is much smaller compared to the absorption of the fundamental vibrations, their detection is challenging. Here, a silicon rib waveguide structure is proposed for label-free on-chip overtone spectroscopy in near-infrared. Our spectrometer distinguished several organic liquids such as N-methylaniline and aniline without any surface modification.

1. Introduction

Silicon photonic devices are made using existing semiconductor fabrication techniques. Since silicon is already used as the substrate for most integrated circuits, it is beneficial to study the guided light and matter interaction with Silicon-On-Insulator waveguides which are operating in near-infrared (near-IR).

It has been shown experimentally[1] and validated theoretically[2] that a waveguide scheme can be efficiently utilized for detection of molecular overtones. Therefore, despite the fact that the cross section of vibrational transitions overtones are few orders of magnitude smaller than that of the fundamental transitions which correspond to the same degree of freedom, overtones and combination modes can be studied on waveguides in near-IR absorption bands and enables identification of multiple bonds in the analyte. Although sophisticated on-chip spectrometers have been demonstrated in mid-IR and near-IR, broadband near-IR spectrometers have never been shown for detection of molecular vibrations overtones with silicon nanostrip. We present a chip-scale photonic device that utilizes near-IR absorption by molecular overtones vibrations for label-free chemical sensing. We designed a multimode silicon nanostrip rib waveguide in such a way that launching the high-order modes improves the sensitivity of the chip-scale device for broadband detection.

2. Results and Discussion

Figure 1 shows the energy levels calculated by Morse potential function for the anharmonic oscillator where ν_f is the fundamental frequency.

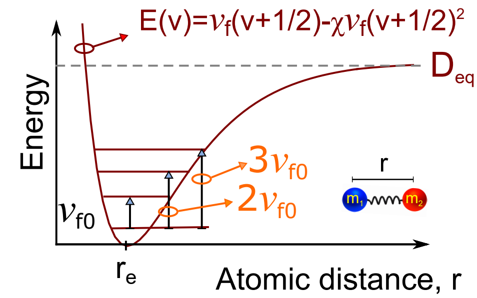

Figure 1: Diagram of an oscillator mechanism described by the energy levels for anharmonic vibration.

The proposed structure, shown in Figure 2, is a nanostrip rib waveguide made of silicon on silica substrate, a height of 2 μm and strip height of 400 nm.

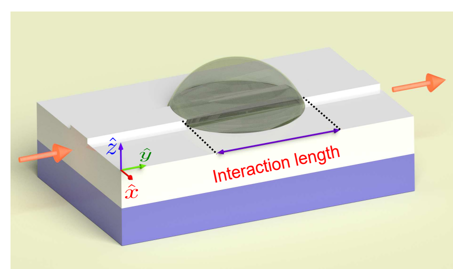

Figure 2: Illustration of the Si nanostrip rib waveguide.

Using Lumerical FDTD, we studied the modes and their absorption for rib waveguide at wavelength of 1.5 μm. Higher order modes have greater absorption in this wavelength due to the strong evanescent field. It is important to understand the evolution of the modes due to the abrupt discontinuity in the medium where the nanostrip is embedded.

Figure 3 shows the cross-sectional colormaps of the evolution of normalized mode profiles exhibiting interference and guidance in the interaction length of the designed waveguide (Figure 2b).

We performed a systematic experimental study where we utilize the enhanced interaction of multimode SOI (Silicon-On-Insulator) rib waveguides with molecular media. We illuminate the waveguides with broadband source butt-coupled to the facet. A pure probe molecules and dilutions with hexane are dripped onto the waveguide surface.

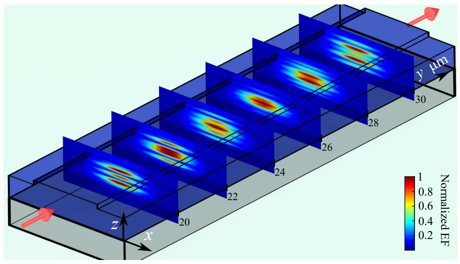

Figure 3: Evolution of the interfered guided modes in the interaction length with the analyte.

Differential transmittance is evaluated from the collected signals, then analyzed and compared to literature values.

Figure 4 shows the experimental results performed on silicon nanostrip rib waveguides.

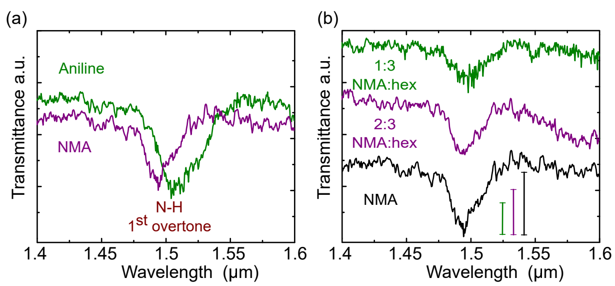

Figure 4: (a) Transmittance spectra of N-methylaniline and aniline. (b) Transmittance spectra of pure N-methylaniline molecule and mixture ratios of 1:3 and 2:3 of N-methylaniline in hexane.

Figure 4a clearly shows the waveguide's ability to distinguish between N-methylaniline and aniline. It shows the absorption of the first overtone of N-H bond of N-methylaniline and aniline around 1.5 μm. In addition, we observed the blue shift in the absorption band between the molecules and the broadening in the N-H first overtone absorption on aniline. Figure 4b shows the transmittance for different mixtures of N-methylaniline and hexane. A lower concentration of N-methylaniline in the sample decreases the absorption, allowing distinguishing between the concentration.

The molecular fingerprints of probe molecules from their overtone absorption spectra were successfully demonstrated with silicon waveguides in near-infrared. This is surprising, since at normal incidence, considering the same interaction length and longer the molecule and their mixtures were not detected. The coupling efficiencies (from fiber to waveguides) including the insertion and propagation losses are -30 dB. Even obtaining such a high loss, the molecular signatures overtones were detected.

3. Conclusions

In conclusion, we proposed a silicon nanostrip rib-waveguide structure for label-free on-chip overtone spectroscopy in near-IR. We show that utilizing the large refractive index contrast ($\Delta n > 2$) between the Si core of the waveguide and the SiO_2 substrate, a broadband near-IR lightwave can be efficiently guided. In addition, we show that the sensitivity for chemical detection is increased by more than 3 orders of magnitude when compared to the evanescent-wave sensing predicted by the numerical model. Our on-chip spectrometer distinguishes between several common organic liquids such as N-Methylaniline and Aniline precisely without any surface modification through the spectral scanning over the absorption dips in the near-IR transmission spectra. The planar near-IR silicon nanostrip waveguide is a compact sensor which can provide a platform for accurate chemical detection. Our near-IR silicon nanostrip rib waveguide device can enable the development of sensors for remote on-site chemical monitoring.

Acknowledgment

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References

[1] A. Karabchevsky and A. V. Kavokin. Giant absorption of light by molecular vibrations on a chip, *Scientific reports* 6 (2016).

[2] A. Katiyi and A. Karabchevsky, Figure of merit of all-dielectric waveguide structures for absorption overtone spectroscopy, *Journal of Lightwave Technology* 35.14 (2017): 2902-2908.