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Planar integrated plasmonic mid-IR spectrometer

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ABSTRACT

A compact spectrometer-on-a-chip featuring a plasmonic molecular interaction region has been conceived, designed, modeled, and partially fabricated. The silicon-on-insulator (SOI) system is the chosen platform for the integration. The low loss of both silicon and SiO₂ between 3 and 4 μm wavelengths enables silicon waveguides on SiO₂ as the basis for molecular sensors at these wavelengths. Important characteristic molecular vibrations occur in this range, namely the bond stretching modes C-H (Alkynes), O-H (monomeric alcohols, phenols) and N-H (Amines), as well as CO double bonds, NH₂, and CN. The device consists of a broad-band infrared LED, photonic waveguides, photon-to-plasmon transformers, a molecular interaction region, dispersive structures, and detectors. Photonic waveguide modes are adiabatically converted into SPPs on a neighboring metal surface by a tapered waveguide. The plasmonic interaction region enhances optical intensity, which allows a reduction of the overall device size without a reduction of the interaction length, in comparison to ordinary optical methods. After the SPPs propagate through the interaction region, they are converted back into photonic waveguide modes by a second taper. The dispersing region consists of a series of micro-ring resonators with photodetectors coupled to each resonator. Design parameters were optimized via electro-dynamic simulations. Fabrication was performed using a combination of photo- and electron-beam-lithography together with standard silicon processing techniques.

INTRODUCTION

Surface Plasmon Polaritons (SPP), inhomogeneous electromagnetic waves tightly confined to the surface of conductors, provide intense localized electromagnetic fields and a potential means information transport in nano-photonic applications. This work investigates the integration of plasmonic elements with silicon photonics to provide a chip scale chemical sensor and spectrometer compatible with CMOS fabrication technology [1].

Silicon on insulator (SOI) waveguides direct mid-IR light to an analyte interaction region, where surface plasmons are generated in metallic slot waveguides to pass through, and be selectively absorbed by, adsorbed chemical species. Efficiently reconverted back to photonic waveguide modes, the transmitted IR optical field is then spectrally analyzed by an array of ring-resonators and integrated detectors. The targeted short wave infrared SWIR region (3 - 4 μm wavelengths) features low loss propagation in silicon and the characteristic absorptions of (e.g.) C-H

(Alkynes), O-H (monomeric alcohols, phenols), N-H (Amines), CO double bonds, NH₂, and CN, as shown in Figure 1. This motivates the shift to longer wavelengths from telecom bands, where the first work waveguide-to-plasmon modes using tapered waveguides was done [2].

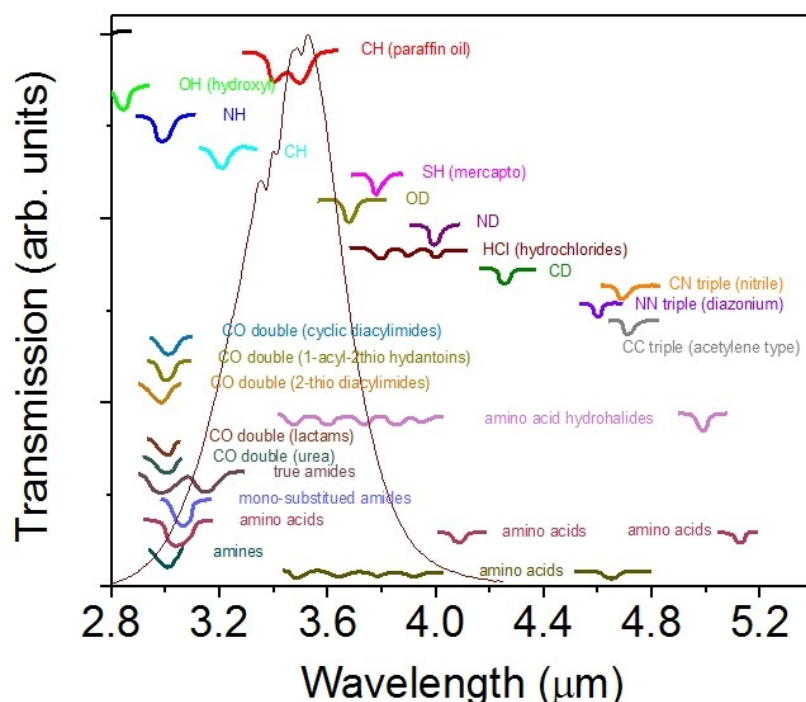


Figure 1 Representative spectra of molecules superimposed on the measured spectrum of a 3.4 μm LED.

Although proposed several years ago, the first experimentally verified transmission of mid-IR radiation through SOI waveguides was published only recently [3]. The authors coupled 3.39 μm radiation from a HeNe laser into a bundle of single mode fibers which were butt coupled to their SOI waveguides. The use of ring resonators as frequency selective elements has also been verified in the mid-IR suggesting their usefulness in this proposed application [4, 5].

EXPERIMENT

IR spectrometer design

Fig. 2 presents a design schematic consisting of source, interaction, and detector regions. A commercial 3.4 μm wavelength LED with ~ 400 nm bandwidth is proposed for use as the optical source which will be coupled into a silicon-on-insulator waveguide adiabatically tapered to a dimension below cutoff, in order to transform the waveguide mode to a plasmon that propagates in the metallic slot of the interaction region shown schematically in Fig. 2b. Molecules will interact with the bound electromagnetic waves in this region, giving rise to absorption. Functionalizing the surface in the interaction region will allow concentration of the molecular analyte in order to measure the infrared absorption of the bound molecules as well as to probe their binding kinetics. After conversion back to a waveguide mode via another adiabatic taper, wavelength dispersion is accomplished through the use of a series of microring resonators.

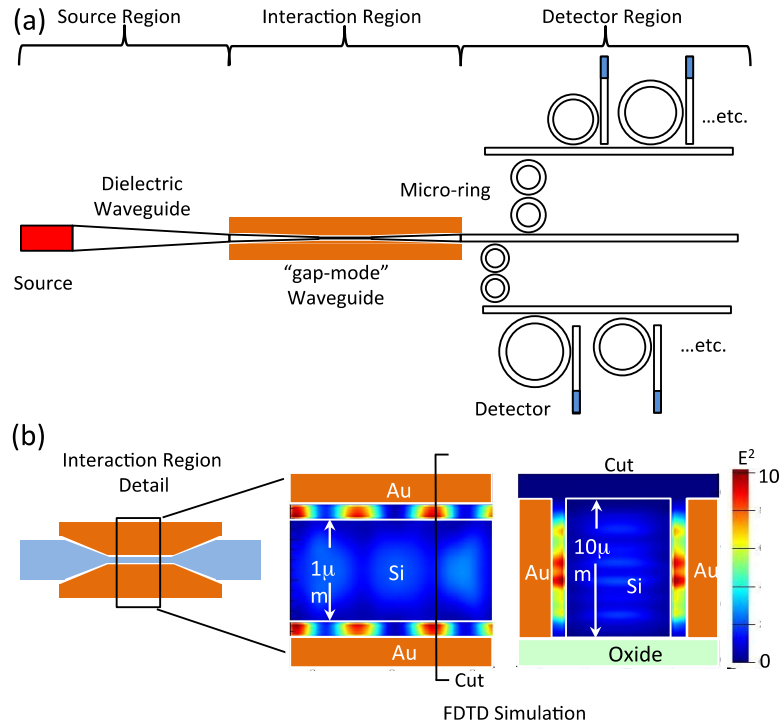


Figure 2(a) Schematic of planar integrated plasmonic mid-IR spectrometer. A broad band LED source feeds a plasmonic based interaction region. The layered micro-ring resonator section as described in the text determines spectral content. (b) FDTD simulation of the interaction region showing generation of plasmon modes in the gap located between the dielectric and the surrounding metal.

Micro-rings resonate when the round trip path length of the optical field is an integral multiple of the effective wavelength of the optical field [4]. The separation between resonances, or the free spectral range, FSR, is inversely proportional to the round trip path length, while the full width half max, FWHM, of any resonance is proportional to the FSR. Decreasing the resonant line width by increasing the round trip path length correspondingly reduces the FSR. Attempts to increase resolution by decreasing the FWHM of the filter resonance introduce ambiguities in wavelength determination if the excitation bandwidth exceeds the FSR. To alleviate this problem, a layered micro-ring resonator approach is proposed (Fig. 2a). The first layer of filters has a small optical path and its FSR needs only to exceed the LED bandwidth. The second layer of filters has a larger optical path length with a reduced FSR that only needs to be as wide as the first layer's FWHM. This second layer will have a correspondingly smaller FWHM and provides the resolution needed for chemical identification. This results in unambiguous determination of the spectral content. Light is coupled from the secondary rings to on-chip detectors (blue elements, Fig. 2a) via an additional set of waveguides (vertical bars, Fig. 2a).

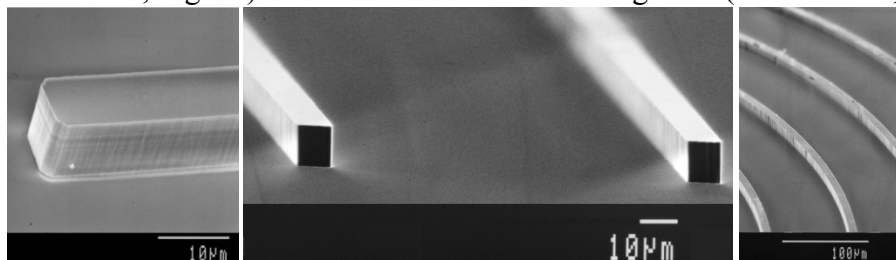


Figure 3 (left) Si waveguide on insulator, (center) Two adjacent Si waveguides 100 μm apart, (right) Bent Si waveguides with different radii of curvature.

Silicon waveguides have been fabricated by reactive ion etching (RIE) with Fluorine chemistry using photolithographically defined metal masks. Fig. 3 presents SEM images of some our waveguides. Vertical sidewalls as well as smooth etched surfaces were achieved.

Interaction region

Fig. 4 presents our process for patterning the interaction region. Electron-beam lithography is followed by metal evaporation and lift-off to form an etch mask (a). The Si top layer is etched using deep RIE, leaving the waveguide structure on top of the oxide layer. A seed layer of ~50 nm of Au is then deposited over the entire area (b), followed by a CVD layer of nitride (c). Conformal coating on the waveguide sidewalls defines the eventual width of the plasmon slot waveguide. Next, the surface is spin-coated with a thick layer of photoresist and a rectangular window opened by lithography (d). The thickness of this resist layer matches or exceeds the height of the waveguide (10 μm). The nitride is etched by anisotropic RIE (e) to remove Nitride from the horizontal surfaces without removing nitride from the vertical sidewalls. This step is followed by electroplating 10 μm of Au over the window (f). The electrical isolation of the waveguide from the rest of the structure in the window should prevent plating of the top of the waveguide. We then strip the resist (g) and wet etch the Nitride from the sidewalls (h). The thin seed layer of Au is then removed and we are left with the tapered interaction region waveguide separated from the metal plasmon host by a gap of the proper width (i).

FDTD simulations of the interaction region are show in Figure 2 b. The cross section is a top down view of the waveguide in the interaction region. As the lateral dimension is tapered to a width of 1 μm , the waveguide becomes too narrow to support a waveguided photonic mode, so the electromagnetic energy is forced into the gap where it excites a SPP bound to the metal. The cross section view displayed in the lower right hand corner is a head on view in the propagation direction through the waveguide.

An estimate for the necessary length of the interaction region may be obtained by simulating the effect of changing the index in the slot. The relevant parameters are the refractive index, the thickness of the layer, and the extinction coefficient. Alternatively, we may estimate the ratio of transmitted optical intensity, I , to source intensity, I_0 , as function of length of using the Beer-Lambert law,

$$\frac{I}{I_0} = T = e^{-\sigma N x} \quad (1)$$

where σ is the absorption cross section, N is the number per unit volume of absorbing molecules. Small ligands (<300 Da) can have characteristic lengths on the order of 10 Angstrom, while 60 kDa biomolecules can be 10's of nm in length. The diameter of the DNA double helix is roughly 2 nm, but of course the length is orders of magnitude larger. Taking as an example a molecule of 10 nm radius gives a molecular volume of 10^{-18} cm^3 , or for 100% concentration, 10^{18} molecules per cm^3 . Estimating an absorption cross section of 10^{-18} cm^2 gives $T = e^{-x}$. (This value of effective cross section for infrared absorption is typical of the 4.7 micron wavelength absorption of CO and more than 10x smaller than the cross section for CO₂ at 4.2 micron wavelength). Thus, for an easily measurable change in transmittance due to molecular absorption of 10%, $x = -\ln(0.9) = 1 \text{ mm}$ is obtained suggesting an appropriate interaction region length of 1 mm. The

propagation length of surface plasmons on gold at 3 micron wavelength is several millimeters [6]. So, sufficient throughput and sufficient path length for sensing are simultaneously feasible.

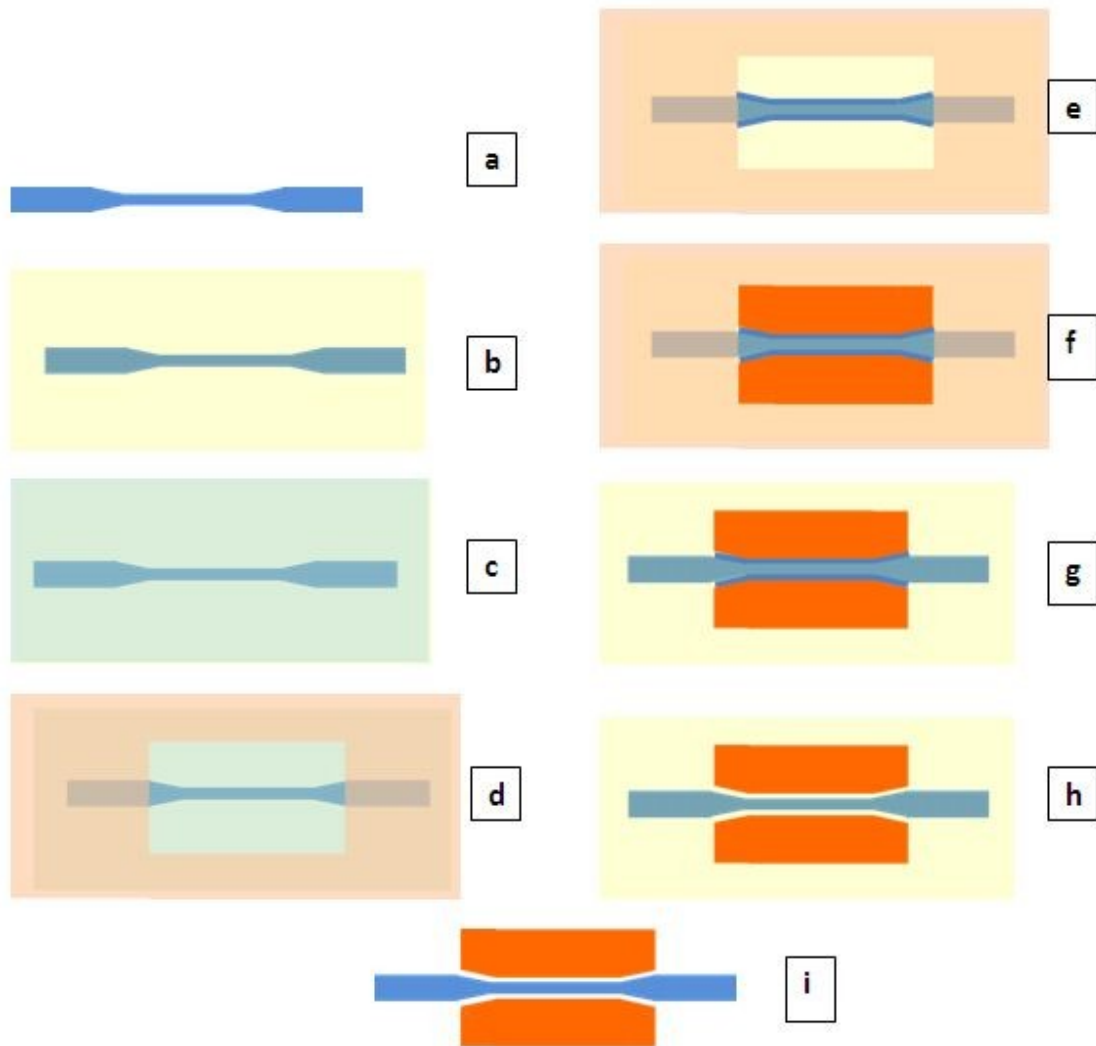


Figure 4: (a-i) Processing steps for fabrication of the interaction region.

Ring resonators

The micro-ring resonators to be defined by e-beam lithography will have widths of approximately $1\ \mu\text{m}$, with distinct channels defined by differences in diameter of tens of nanometers. As an example, a first layer of micro-ring resonators with $1.58\ \mu\text{m}$ diameters might be used with a second layer of $15.82\ \mu\text{m}$ diameters, where their resonance FWHM of roughly $3\ \text{nm}$ would be suitable for chemical identification in the SWIR as proposed. All dimension are well within the range of ebeam lithography and are approaching dimensions whereby optical lithography could be used throughout for the fabrication of this integrated nanophotonic chip. To cover the entire 3-4 micron emission bandwidth of the IR LED (Fig. 1) would require approximately 300 of the 3-nm-resolution secondary rings.

CONCLUSIONS

A chip scale method of molecular sensing based on surface plasmon resonance in mid-IR range has been designed and partially fabricated. Existing systems of this type operate at visible wavelengths, but the region around 3.4 μm wavelength offers potential advantages in sensitivity and selectivity based on characteristic molecular absorption and dispersion. Our approach involves fabrication of a chip-scale spectrometer with a surface plasmon enabled molecular sensing region and multi-layered, micro-ring resonator filters for the determination of spectral content.

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