Design of Cavity-Enhanced Photothermal Mid-Infrared Spectroscopy for Sensing Applications

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A design is presented which combines the mature Silicon-On-Insulator (SOI) platform at telecom wavelengths with the ultra-sensitive and selective photothermal spectroscopy for miniaturized sensing applications. Organic based materials all exhibit a distinct "fingerprint" region in the mid-infrared (3-4 μm) part of the absorption spectrum $\alpha(\lambda)$ *which can be probed using a tunable mid-infrared source. Absorption gives rise to a temperature change which changes the real part of the refractive index through the thermo-optic effect. Simulations show that localization of thermal and optical interactions allows for a very sensitive and compact measurement method.*

Introduction

The Silicon-On-Insulator (SOI) platform is a mature CMOS-compatible technology that has paved the way for a myriad of telecom applications [1] and this portfolio is now rapidly expanding towards miniaturized sensing applications such as label-free biosensing [2] and gas sensing [3].

Spectroscopic sensors are an important and industry relevant class of devices that probe the unique "fingerprint" absorption spectrum of molecules $\alpha(\lambda)$. These sensors are unmatched in terms of selectivity for rapid label-free detection of chemical components in a mixture. The mid-infrared wavelength region is of particular interest due to the higher optical absorption at these frequencies and hence lower limit of detection (LOD). However, these type of sensors for the mid-infrared are typically bulky and expensive and therefore quite some work is geared towards the integration and miniaturization of various optical components for this wavelength range [4].

Photothermal spectroscopy methods are a class of highly sensitive and selective approaches that measure the optical absorption of materials indirectly. The optical absorption $\alpha(\lambda)$ induces a change of the thermodynamic parameters: pressure, density and temperature which can be probed independently from the excitation source. These techniques have proven to be extremely sensitive and robust to environmental noise for the detection of various chemical compounds. LOD values of parts-per-trillion (ppt) have been demonstrated [5]. One major disadvantage of scaling down this type of sensor is that the optical interaction path length is reduced proportionally, degrading the sensitivity of the device. To counteract this, enhancement effects have to be implemented to obtain the same performance levels of bulky, high-cost instruments [6]. Here we analyze a possible implementation of photothermal mid-infrared spectroscopy in the SOI platform. This approach circumvents the need of a costly and cooled mid-infrared detector and enhances the photothermal signal using a high Q microring resonator.

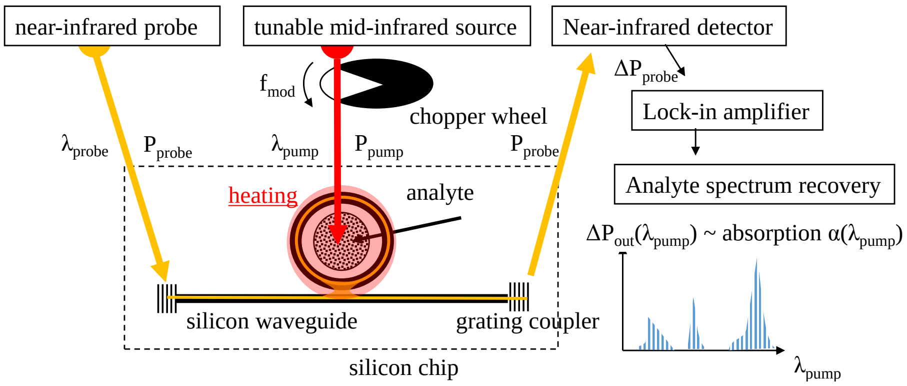


Figure 1: Possible measurement setup for photothermal spectroscopy. The tunable mid-infrared pump laser is scanned across the absorption spectrum of the analyte. The generated heat is transduced to a change Δn_{eff} and then ΔP_{probe} using a high Q ring resonator which is then detected using a cheap near-infrared system. The modulation depth, proportional to the infrared absorption at λ_{pump}, is sensitively read-out using a lock-in amplifier.

Photothermal signal model

The analyte is deposited or captured in the annular regioin of the microring resonator by means of a patterned functionalization layer on top of the silicon chip. The wavelength selective absorption of mid-infrared radiation by the analyte will give rise to a wavelength selective temperature increase $\Delta T(\lambda_{pump})$ which is transferred to the resonator. The increase in temperature causes a change of the effective refractive index n_{eff}. The change Δn_{eff} is read out by a near-infrared probe coupled to the ring resonator. This shift is transduced to a power change ΔP_{probe} of the detected probe signal. The probe wavelength λ_{probe} is chosen at a point where the transmission spectrum has the highest slope $d\mathcal{T}/d\lambda = \mathcal{T}'$. By modulating the heating mid-infrared pump beam, the wavelength shift will translate into a modulated probe power change $\Delta P_{probe}(\lambda_{pump})$ which can be read out sensitively using a lock-in type detection. A sketch of a possible setup is given in Figure 1. The small signal modulation ΔP_{probe} is given by

$$\Delta P_{probe} \approx P_{probe,max} \frac{d\mathcal{T}}{d\lambda}(\lambda_{probe})\Delta\lambda$$

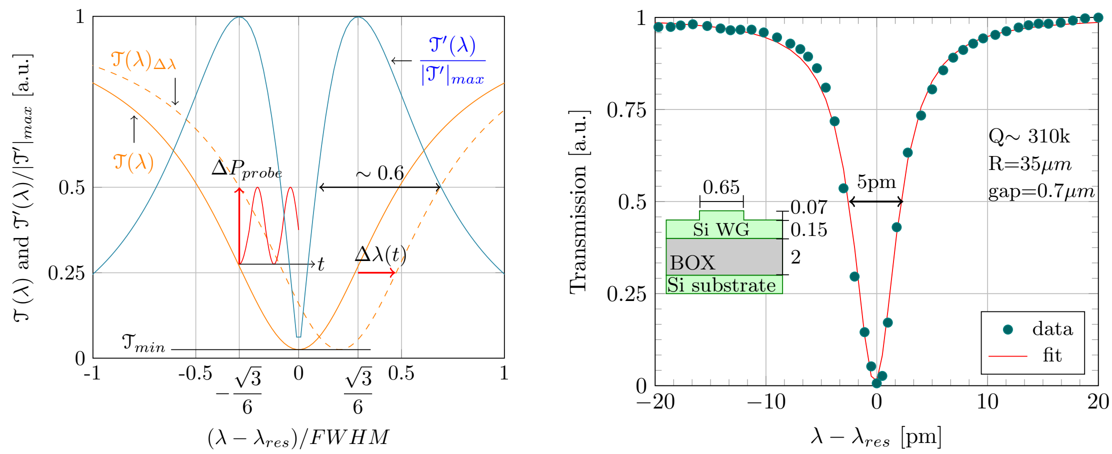
with $\mathcal{T}(\lambda)$ the Lorentzian approximation of the normalized all-pass ring transmission spectrum near resonance [7]. ΔP_{probe} is maximal when the probe wavelength is tuned to $\lambda = \lambda_{res} \pm FWHM\frac{\sqrt{3}}{6}$ where

$$|\mathcal{T}'|_{max} = (1-\mathcal{T}_{min})3\sqrt{3}/(4FWHM) = (1-\mathcal{T}_{min})3\sqrt{3}Q/(4\lambda_{res})$$

with $FWHM$ the Full Width at Half Maximum and Q the loaded quality factor $Q \approx \lambda_{res}/FWHM$. The resonance wavelength shift $\Delta\lambda$ due to temperature increase ΔT is given by [7].

$$\Delta\lambda = \frac{\lambda_{res}}{n_{eff}}\left(\frac{\partial n_{eff}}{\partial T}\Delta T + \frac{\partial n_{eff}}{\partial \lambda}\Delta\lambda\right) + \lambda_{res}\varepsilon\Delta T$$

with $\partial n_{eff}/\partial T$ the thermo-optic coefficient of silicon, $\partial n_{eff}/\partial \lambda$ the material dispersion and ε the thermal expansion coefficient. In silicon, ε is two orders of magnitude lower



(a) (b)

Figure 2: Normalized Lorentzian transmission model $\mathcal{T}(\lambda)$ and derivative $\mathcal{T}'/|\mathcal{T}'|_{max}$ of an all-pass ring resonator, indicating the optimal probe position where ΔP_{probe} is maximal. (a) Measured high-Q all-pass ring resonance at 1550 nm in the SOI-platform with ring radius R=35μm and coupling gap of 0.7μm. (b) The inset shows the waveguide cross-section, all dimensions are in μm.

than the thermo-optic coefficient. Together with the definition of the group index n_g this reduces to

$$\Delta\lambda = \frac{\lambda_{res}}{n_g}\frac{\partial n}{\partial T}\Delta T$$

The temperature increase of the ring resonator is estimated by using the Lambert-Beer absorption law for low absorption

$$\Delta T = \gamma P_{abs} R_{th} = \gamma P_{pump} R_{th} \alpha(\lambda_{pump}) L$$

with γ the fraction of optically absorbed power converted to heat, P_{pump} the incident mid-infrared pump power, L the effective optical interaction path length of the pump with the analyte, R_{th} the effective thermal resistance of the ring resonator in K/W and $\alpha(\lambda_{pump})$ the analyte-specific absorption coefficient in m^{-1}. Assuming that the linewidth of the scanning pump laser is much broader than the absorption features of the analyte, we estimate the maximum probe signal change at a chosen absorption peak wavelength $\alpha(\lambda_{pump})$ as

$$|\Delta P_{probe}|_{max}[\alpha(\lambda_{pump})] = \frac{3\sqrt{3}(1-\mathcal{T}_{min})}{4n_g}\frac{\partial n}{\partial T}\gamma Q R_{th} P_{probe} P_{pump} L \alpha(\lambda_{pump}) \qquad (1)$$

Thermal analysis and limit of detection

To evaluate the performance of this design, one must find a reasonable estimate of the parameters in eq (1). The thermo-optic coefficient for Si is known to be $1.8 \times 10^{-4} K^{-1}$ and $n_g \sim 4$. Example of a high Q (300k) ring resonator is shown in Figure 2(b), $\gamma \sim 1$, $\mathcal{T}_{min} \sim 0$ and we assume a moderate mid-infrared pump power of 10 mW focused onto a ring with 25μm radius. The effective optical absorption path length L for a functionalized chip is taken around 10μm. It is not trivial to estimate the noise levels of a lock-in type detection scheme which will depend on the complete setup configuration.

Here we propose a safe, practical value for the minimal detectable probe signal change $|\Delta P_{probe}/P_{probe,max}|_{min} \sim 10^{-4}$. The thermal resistance R_{th} is estimated using a Finite Element Method (FEM) in *COMSOL*. The steady state temperature distribution is calculated for heat generated inside the annular region of the resonator. The average temperature increase in the waveguide cross-section is evaluated yielding a thermal resistance R_{th} of ∼400 K/W. Using these values, minimal absorption value is estimated $\alpha_{min} \sim 10^{-3} cm^{-1}$. Typical absorption values for gases are of the order $\alpha_{gas} \sim 5 \times 10^{-5} ppm^{-1} cm^{-1}$ [6]. This implies a limit of detection (LOD) of 20 ppm. However, simulation results in Figure 3 show that by locally etching away the silicon substrate from the backside of the chip, one can improve the thermal resistance up to 10^4 K/W, which would bring the LOD down to sub-ppm concentrations.

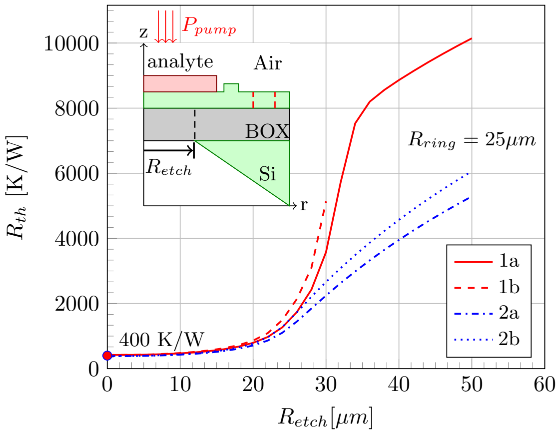


Figure 3: FEM simulation of R_{th} for thermally isolated rings for different backside Si-openings R_{etch}. The ring is further thermally isolated by dry etching an opening in the top Si, as depicted by the red dashed lines in the inset, results: (1a,1b). Additionally we can also etch away the BOX underneath the ring, results: (1b,2b).

Conclusion

The proposed photothermal spectroscopy design leverages the low-cost, high volume SOI-platform for future miniaturized mid-infrared spectroscopy applications. High Q ring resonators enable small footprint passive transducers, cancelling the need for expensive, cooled mid-infrared detectors. Thermal FEM simulations show that by locally under etching the structures the estimated LOD can be brought below 1 ppm.

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