Light-on-a-Chip Group
Electrooptical Engineering

BGU

Light-Overtones Interaction with Guided Wave Optics Scheme

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Overview

Project aim

- The project focuses on exploiting the near-infrared absorption enhancement by overtones with guided wave architectures due to enhanced light-matter interaction.

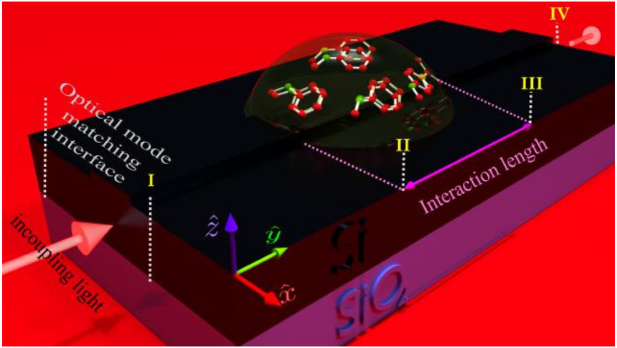


Figure 1: The concept.

Mid-infrared spectroscopy

- Mid-infrared (Mid-IR) spectroscopy is powerful technique for molecular detection.
- The absorption spectra of organic molecules, in this region, are directly linked to the fundamental vibrational modes.
- A fundamental vibrational transitions of organic molecules are typically in range of 3-20 μm or in wavenumbers it is ~3300-500 cm^{-1}.
- Infrared absorption spectroscopy exhibits a great potential in sensing and molecular dete

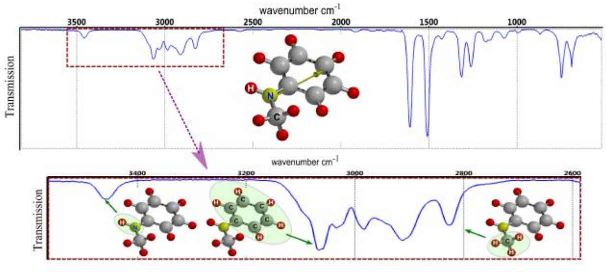
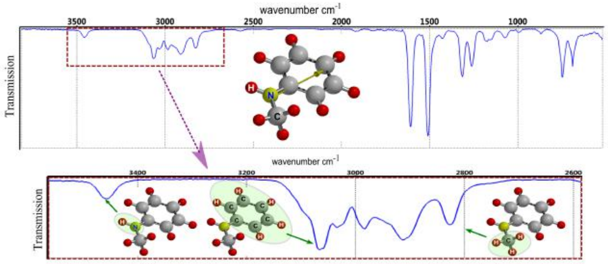


Figure 2: Calculated MIR spectrum of N-Methylaniline molecule using Spartan computational chemistry software.

Mid-infrared spectroscopy

- Theoretically, spectroscopic transitions occur at absorption lines with zero frequency width.
- Absorption lines with finite widths and characteristic lineshape functions, directly related to the absorption coefficient and dielectric function of the molecule.
- Well defined absorption band in mid-ir region are related to molecular fingerprints due to the large absorption cross-section.
- Despite their potential, the fundamental vibrations of organic molecules appear in mid-infrared region where bulky and expensive equipment is needed.



Our approach

Quick look into the lab:

- Our approach is the investigation of absorption by overtones in the near-infrared region using guided wave optics.
- Telecommunication region has affordable equipment due to the technological maturity at this window.
- The use of chip allows for light-matter interaction in a controllable manner harnessing the miniaturization and portability.

(a) (b)

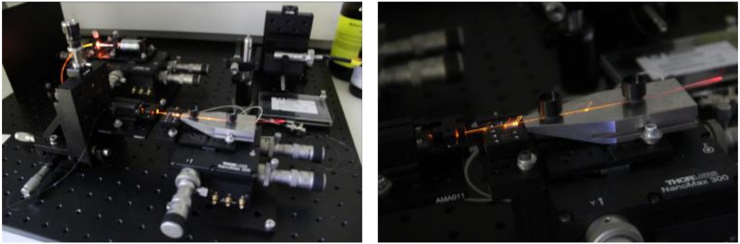


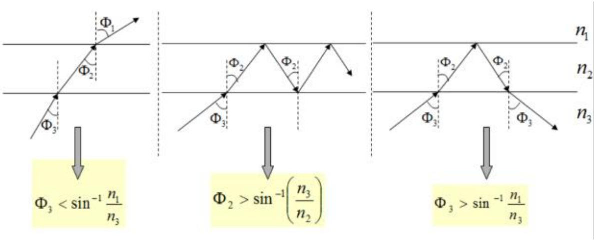
Figure 3: (a) The experimental set-up; (b) Examined chip.

Guidance principle

- In a guided wave optics regime, the guiding layer has a higher index than the surroundings which allows the wave propagates due to total internal reflection.

$$\theta_c = \sin^{-1}\left(\frac{n_{\mathrm{subs}}}{n_{\mathrm{gl}}}\right) \quad (1)$$

$$n_{\mathrm{gl}} > n_{\mathrm{subs}} \geq n_{\mathrm{sups}} \quad (2)$$



$$\beta_m = k n_{\mathrm{gl}} \cdot \sin(\phi_2) \quad (3)$$

Guidance criterion

- We solve the wave equation to find the (a) guiding modes, (b) propagation constants and (c) effective indices.

$$(\nabla^2 + \beta^2)E(x, y) = 0 \quad (4)$$

$E_y(x)$	Domain
$Ae^{-q(x-d_g)}$	$d_g \leq x \leq \infty$
$B\cos(hx) + C\sin(hx)$	$0 \leq x \leq d_g$
De^{-px}	$-\infty \leq x \leq 0$

- For guided mode, the effective index of the mode needs to follow the criterion:

$$n_{\text{subs}} \leq n_{eff} \leq n_{\text{gl}} \qquad n_{eff} = \beta_m / k \quad (5)$$

Eigenfunctions

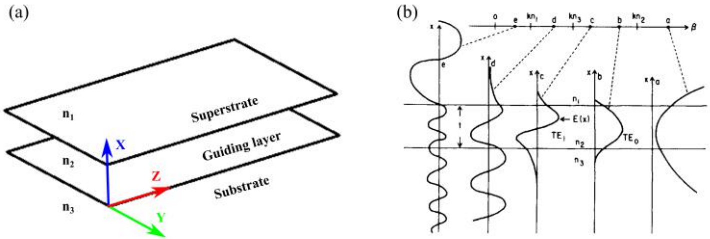


Figure 4: (a) Slab waveguide. (b) Possible modes in a slab waveguide[1].

- The part of the mode which propagates beyond the guiding layer is named the evanescent field. This field can interact with the surrounding within penetration depth interval.

[1] Robert G. Hunsperger, "Integrated Optics"

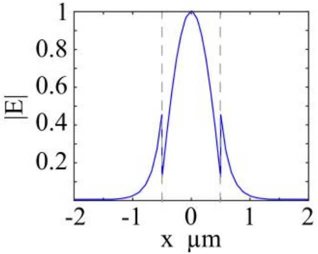
Evanescent field

- The evanescent field is the fraction of power which propagates beyond the guiding layer and defines the FoM.

$$\text{FoM} = \eta_{\text{evanes}} = \frac{P_{\text{evanes}}}{P_{\text{total}}} = \frac{\int_{\text{medium}} S dA}{\int_{-\infty}^{\infty} S dA} \quad (6)$$

$$S = \frac{1}{2}\Re\{E \times H^*\} \quad (7)$$

S - Poynting vector
P - Power
E - Electric field
H - Magnetic field
$\Re$ - Real part
A - Area



Waveguide architectures

- The FoM of common waveguide architectures were studied.

A. Katiyi and A. Karabchevsky, Journal of Lightwave Technology. 2017;35(14):1-7

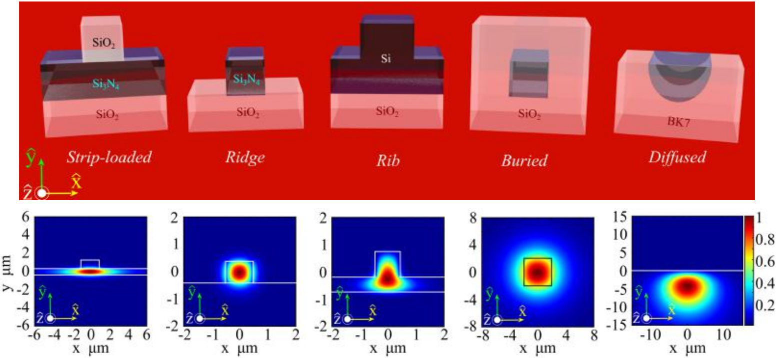


Figure 5: (Top) Common single mode waveguide architectures with (Bottom) normalized electric field amplitude colormaps.

Evanescent field in single mode waveguide

- With single-mode operation, the evanescent field is too small for sensing.

Table 1: Fraction of the power carried by the modes of SM waveguides, width of W, embedded in mixture with ratio 1:3 of NMA:Hexane at 1.5 μm.

Waveguide type	quasi-TE		quasi-TM	
	η_{core}	η_{evan}	η_{core}	η_{evan}
Ridge	0.868213	0.0868	0.858926	0.094387
Slab	0.896623	0.050775	0.88289	0.056531
Rib	0.991583	0.004672	0.992465	0.006981
Diffused	0.99819	0.001783	0.998398	0.001603

- Downscaling the physical dimensions of the guiding layer results in increased evanescent field and increased absorption.

Evanescent field in squeeze waveguide

Table 2: Fraction of power carried by the modes at half width of SM waveguides, width of W/2, embedded in molecular mixture at 1.5 μm.

Waveguide type	η_{core}	η_{evan}
Ridge	0.598454	0.323221
Slab	0.883412	0.056531
Rib	0.978077	0.011161
Microfiber	0.67076	0.329247

- The downscaling the physical dimensions of the guiding increases the FoM, as compared with the values summarized in the previous table.
- Ridge waveguide and microfiber show the highest FoM values, which is more than 30%.

Modes in squeeze waveguide

A. Katiyi and A. Karabchevsky, Journal of Lightwave Technology. 2017;35(14):1-7

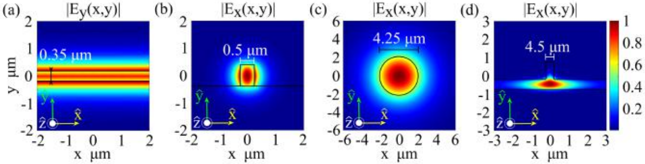


Figure 6: Half width of SM waveguides, width of W/2, embedded in the mixture ratio of 1:3 NMA in Hexane: (a) slab waveguide, (b) microfiber, (c) ridge waveguide, and (d) rib waveguide.

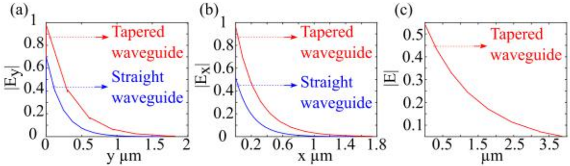


Figure 7: Cross-section of the evanescent field of thin waveguide compared to the monomode waveguides embedded in the mixture. (a) Slab waveguide, (b) Si_3N_4 ridge waveguide on silica, and (c) silica microfiber.

Tapered waveguide architectures

- Tapered ridge waveguide and tapered fiber architectures allow for the enhanced evanescent light-molecule interaction.

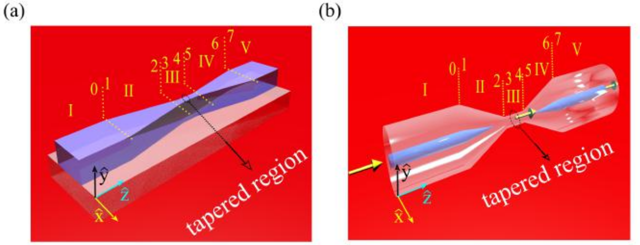


Figure 8: Tapered waveguide architectures: (a) tapered ridge waveguide. (b) microfiber.

Tapered fiber

- In microfiber, the core is too narrow to guide light and the cladding became the guiding medium.
- We investigated the influence of microfiber radii on the mode shape.

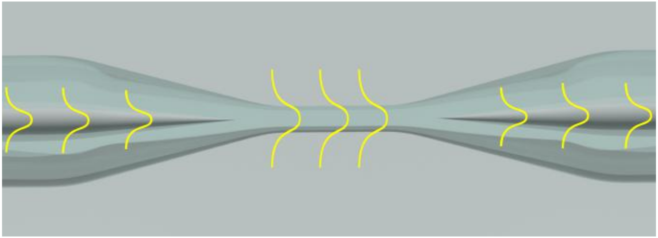


Figure 9: Schematic cross-section of the tapered fiber and the illustration of the propagating mode.

Evanescent field in microfiber

A. Karabchevsky, **A. Katiyi**, et. al., *under review by Light: Science & Applications*.

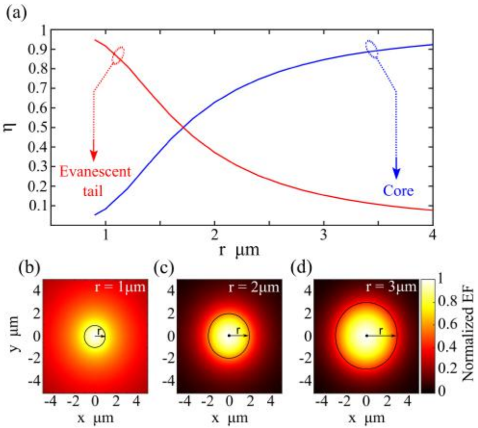


Figure 10: Numerical modelling of microfiber embedded in mixture ratio 1:3 of NMA:Hexane at 1.5 μm with various radii using Comsol Multiphysics.

Vibration overtones

The principle of vibration mechanism

- Each molecule can have 5 types of energy: translational energy, rotational energy, vibrational energy, electronic energy and spin energy.
- Illumination of a molecule in IR spectrum results the molecule to vibrate.
- Each molecule can vibrate in different stretching and bending modes which appear as absorption bands in the IR region.

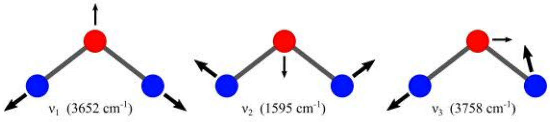


Figure 11: Different vibration modes of H_2O molecule and its excitation frequencies in wavenumber cm^{-1}.

Molecule as an anharmonic oscillator

- Molecular vibration motion is an anharmonic oscillator.
- Anharmonic oscillator energy levels are approximated by Morse potential function.

$$V = D_e[1 - e^{-a(r-r_e)}]^2 \qquad (8)$$

- The frequency which leads to the transition from v=0 to v=1 calls the fundamental frequency.
- The frequencies which result transitions of Δv>1 call overtones.

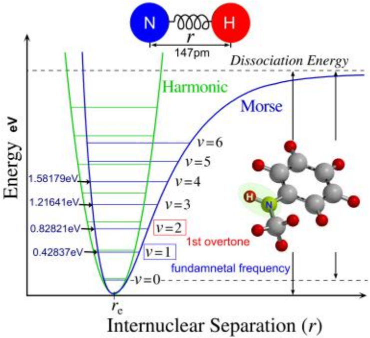


Figure 12: Morse potential function for unharmonic vibration compared to harmonic vibration.

Probing molecules

- Amine, derivative of Ammonia, is widely used in biology and medicine research.
- We study the amine N-H bond in aromatics amines: Aniline and a derivative of Aniline - N-Methylaniline (NMA).
- Mixtures of NMA with Hexane were chosen for checking the ability to distinguish between the different concentrations absorption.

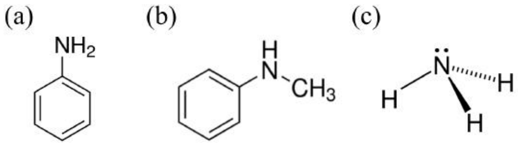


Figure 13: Molecule chemical formula: (a) Aniline $C_6H_5NH_2$ (b) N-Methylaniline $C_6H_5NH(CH_3)$ (c) Ammonia NH_3.

Aromatic amines vibration mode

- Aromatic amines have vibrations mode due to C-H and N-H bonds.
- Aniline C-H first and second overtones are at 1.685 μm and 1.143 μm, respectively. N-H first overtones is at 1.507 μm[2].
- NMA C-H first and second overtones are at 1.683 μm and 1.141 μm, respectively. N-H first overtone is at 1.497 μm.

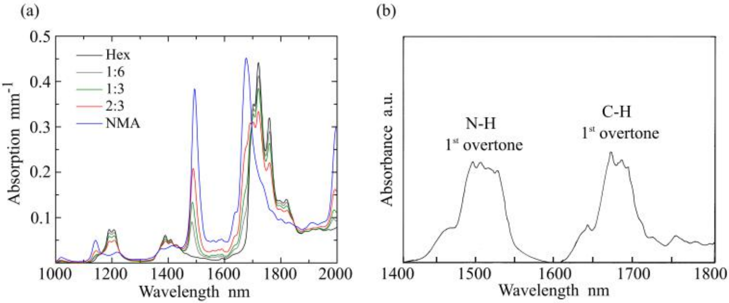


Figure 14: The absorption bands of (a) N-Methylaniline and (b) Aniline

[2] S. Shaji and T. Rasheed, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 57, 337-347 (2001).

Metarials dispersion

- The extinction coefficient κ was measured by using a UV/VIS/NIR spectrophotometer.
- Kramers-Kronig relation was used to calculate the complex refractive index of the samples from the measured κ.

$$\widetilde{n} = n + j\kappa \tag{9}$$

$$n(\omega) - 1 = \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\omega'\kappa(\omega')}{\omega'^2 - \omega^2}\, d\omega' \tag{10}$$

$$\kappa(\omega) = -\frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{n(\omega') - 1}{\omega'^2 - \omega^2}\, d\omega' \tag{11}$$

Metarials dispersion

A. Katiyi and A. Karabchevsky, Journal of Lightwave Technology. 2017;35(14):1-7

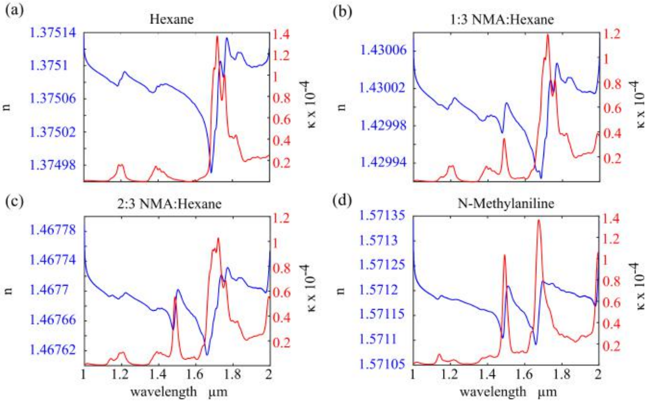


Figure 15: Dispersion of (a) Hexane, (b) ratio 1:3 of NMA:Hexane, (c) ratio 2:3 of NMA:Hexane and (d) pure NMA calculated using KK relation.

Tapered waveguide design

- Tapered ridge waveguide was chosen due to its robustness and inertia to environmental changes.
- Silicon nitride Si_3N_4 was chosen to the guiding layer.
- The guiding layer covers with 1 μm of silica - SiO_2, except for the sensing region.

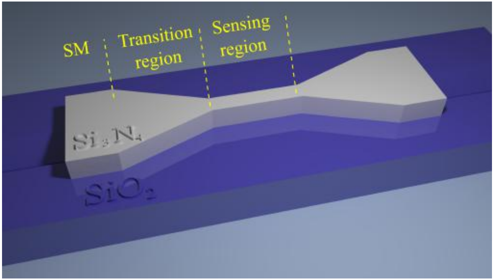


Figure 16: Schematic of the ridge waveguide for the project.

Single mode region

- Single-mode regions were chosen for the input and the output of the waveguide. It allows for easy coupling and easy light collection.
- The fabrication process results guiding layer height of 400 nm.
- The calculated width for SM region was 700 nm.

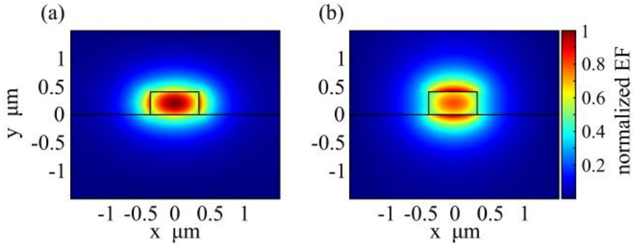


Figure 17: Normalized electric field amplitude. (a) Fundamental TE and (b) fundamental TM in SM ridge waveguide.

Transition region

- There are few tapering architectures: linear, hyperbolic, parabolic and S-type.
- The tapering region needs to be adiabatic to decrease the scattering losses.
- The optimal shape for the tapering is S-shape with a length of 50 μm.

Figure 18: Taper region shapes : parabolic, S-type, hyperbolic and linear.

Sensing area

- The thin region, where the evanescent field increases, is named the sensing area.
- The evanescent field was calculated for NMA and ratio 1:3 of NMA:hexane for wavelengths of 1-1.7 μm.
- The calculated width for the sensing area was 350 nm.

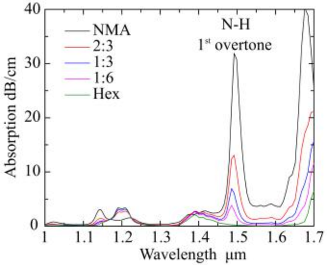


Figure 19: Absorption for different samples with 350 nm width of the sensing region.

Sensing area propagation losses

- The sensing region was simulated with various lengths to calculate the propagation losses by using Lumerical.

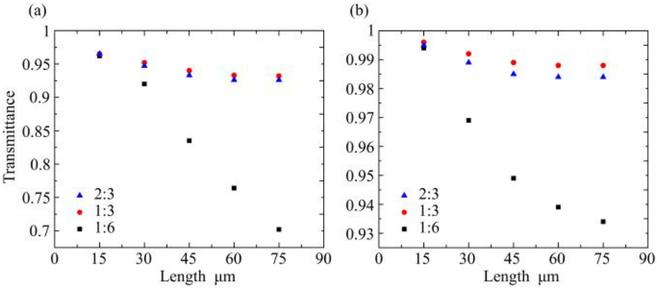


Figure 20: Propagation losses with different guiding layer widths at 1.5 μm: (a) 350 nm (b) 400 nm

- Thinner sensing layer increases the propagation losses and causes the power to leak which limits the variety of samples that can be checked.

Aromatic amines experiment

- Broadband laser source was coupled into the waveguide by single-mode fiber.
- The fiber holds with a piezo-electric stage for precise adjustment of the fiber.
- The output signal was collected by multi-mode fiber into an optical spectrum analyzer.

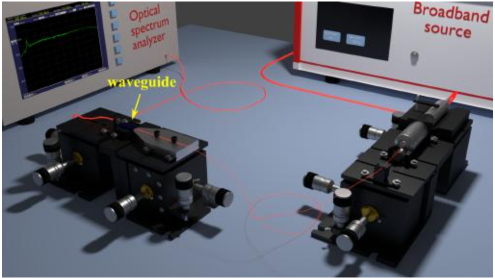


Figure 21: Schematic of the experimental set-up.

Aromatic amines experiment

- We investigated the overtone absorption of aromatic amines using a rib silicon waveguide.
- The samples were Aniline, NMA and mixtures with ratio 1:3 and 2:3 of NMA:Hex with volume of 3 μL.

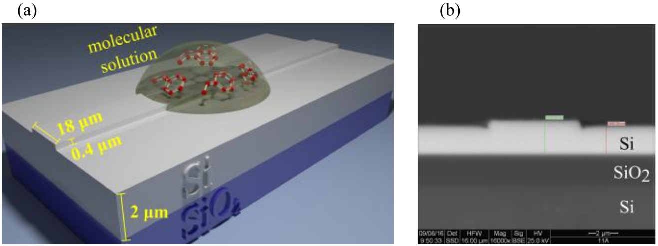


Figure 22: (a) Silicon rib waveguide used in the experiment. (b) Cross section of the rib waveguide by SEM.

Results

- The experimental results clearly show the ability to distinguish between the mixtures and between NMA and Aniline.

A. Katiyi and A. Karabchevsky, Journal of Lightwave Technology. 2017;35(14):1-7

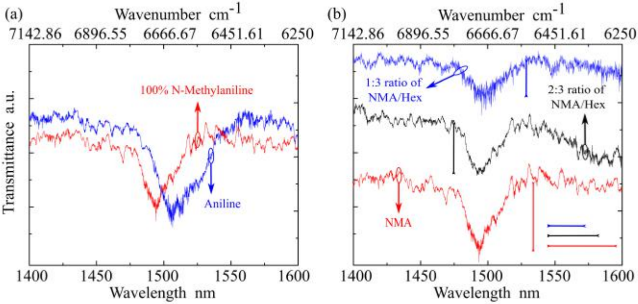


Figure 23: The transmittance spectra of different samples on silicon rib waveguide.

Ovarian cancer experiment

- The experiment was investigating of the spectra changes before and after treatment in ovarian cancer cells.
- The fiber was tapered to approximately 2.5 μm diameter to increase the evanescent field fraction. The fraction is approximately 8-15% due to fabrication tolerance.

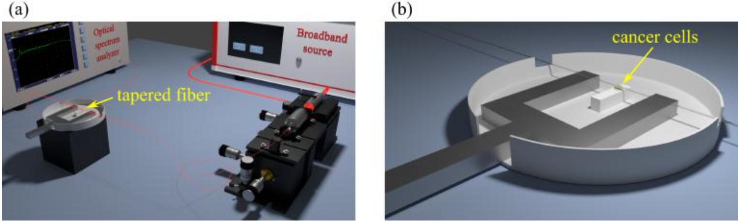


Figure 24: Ovarian cancer experiment. (a) Schematic of the experimental set-up. (b) Microfiber sensing device used in the experiment.

Results

- The experimental results clearly show a difference in the transmittance spectra before and after treatment of 24hr.

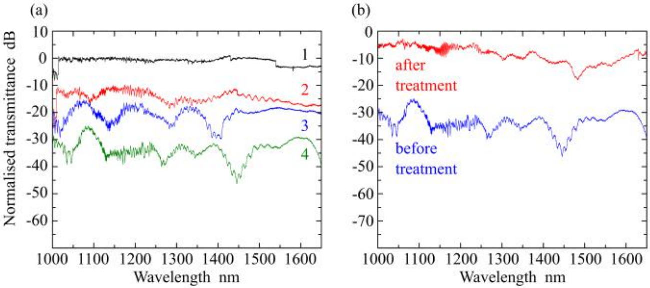


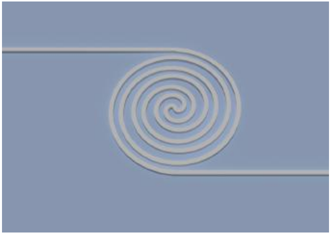
Figure 25: Normalised transmittance: (a) With time difference of 30 sec. (b) Before and after treatment of 24hr.

Conclusion

- We study guided wave architectures for enhanced molecular overtones absorption spectroscopy.
- We showed that tapered structures exhibit an increased evanescent field.
- We investigated tapered structures for overtone absorption in the near-infrared.
- The molecular fingerprints of probe molecules from their overtone absorption spectra were successfully demonstrated with rib silicon waveguides in near-infrared.
- We showed a difference in the transmittance spectra in ovarian cancer before and after treatment of 24hr using microfiber.

Future directions

- Investigate the overtone absorption in the rib waveguide.
- Investigate the difference in the transmittance spectra in ovarian cancer before and after treatment of 24hr.
- Fabricate and investigate the tapered ridge waveguide structure.
- Investigate waveguide with long sensing area for increased absorption.



Summary

Journal articles

[1] **A. Katiyi** and A. Karabchevsky, "Figure of merit of all-dielectric waveguide structures for absorption overtone spectroscopy", Journal of Lightwave Technology, 35(14):1-7 (**2017**).

[2] A. Karabchevsky, **A. Katiyi**, M. I. M. Abdul Khudus and A. V. Kavokin, "Tuning the near-infrared absorption of aromatic amines with photonic microfibers sculptured by electronegative mediators gold nanoparticles", *under review by Light: Science & Applications*.

[3] **A. Katiyi**, B. Hadad and A. Karabchevsky, "Broadband Near-Infrared Spectrometer Using Si Nanostrip Rib-Waveguide for Label-Free On-Chip Chemical Sensing", *in Preparation*.

Conference papers

[1] **A. Katiyi** and A. Karabchevsky, "Nano-tapers: squeezing light in a dielectric nano-guide for overtone spectroscopy", *"Metanano 2016"*, Anapa, Russia, 5 - 9 September 2016. *Invited talk*.

[2] **A. Katiyi**, B. Hadad and A. Karabchevsky, "Silicone Waveguides for Broadband overtone spectroscopy of N-Methylamine and Aniline in near-infrared", *OASIS6*, Tel Aviv, Israel 27-28 Feb 2017.