Enhancement of light absorption, scattering and emission in high index contrast waveguides

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Abstract: The enhancement of absorption/emission or scattering by particles around channel waveguides is calculated. The role of the waveguide refractive index contrast as well as of the core shape is elucidated.
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1. Introduction

In the past years, sensors based integrated photonics has been developed as a very promising route for the lab-on-a-chip sensing applications [1]. A class of sensors is based on waveguide assisted spectroscopic techniques, such as absorption spectroscopy, fluorescence spectroscopy and Raman spectroscopy. These spectroscopic sensors are based on light-matter interaction enhanced by the evanescent field of the waveguide and allow a direct measurement of the specific spectrum of the molecules rather than by other indirect methods, such as in the case of refractive index sensing. The fundamental problem of determining the efficiency of absorption of a waveguide mode by a particle and the subsequent coupling of the emission of this particle to the waveguide mode has only been investigated partially so far [2][3]. The same can be said for Rayleigh and Raman scattering by the particle. The efficiency of absorption and emission depends on the overlap of the particles with the intensity of the evanescent part of the guided mode. On the one hand, higher index contrast and larger core geometry confines light more in the core than in the cladding, thus reduces the effective sensing volume, but, on the other hand higher confinement leads to increased intensity of the evanescent field for a given input power. Hence, the role of index contrast and waveguide geometry on the overall efficiency of linear absorption/emission or scattering processes needs to be clarified. Thus, this problem has to be distinguished from the optimization of optical interactions in the core of the waveguide [4][5].

In this work, we determine the overall efficiency (η) of absorption from a mode and subsequent emitted power coupled to the fundamental quasi-TE and quasi-TM guided modes of a rectangular channel waveguide by uniformly distributed particles in the surrounding. We define η as the ratio between the emission power collected by the molecules and the incident pump power in the mode. As is the case for common sensing scenarios, we distinguish two cases, a) bulk-sensing, where the particles are spread across the whole of the cladding volume, and, b) surface-sensing, where the particles are adsorbed on the waveguide such that they lie within a thin layer around the waveguide (Fig. 1). We will numerically evaluate the overall efficiencies as a function of the normalized waveguide area (A) and aspect ratio (a) for Silicon (n=3.5) and Silicon Nitride (n=2) waveguides in water (n=1.33) cladding.

2. Methodology

An emitter can be modeled as an oscillating dipole, oscillating at frequency c/λ_0. We assume that it is located at the position $\boldsymbol{r_0}$ in the cladding. In semi-classical approach, using Fermi's golden rule, the rate of emission, hence the power coupled to a waveguide mode (P_{wg}) can be calculated to be [5]:
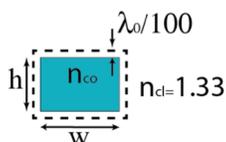

Figure 1: The channel waveguide geometry investigated in this article. Water cladding surrounds a rectangular Silicon or Silicon Nitride channel waveguide. The molecules are suspended uniformly, either all over the bulk of the cladding (bulk sensing) or adsorbed on the waveguide forming a layer of thickness $\lambda_0 /100$ around the waveguide (surface sensing). Aspect ratio a is defined as $a=w/h$.

$$P_{wg}(\vec{r}_0) = P_0 \frac{3}{4\pi} \frac{n_g}{n} \left(\frac{\lambda_0}{n}\right)^2 \frac{\varepsilon(\vec{r}_0)\left|\hat{d} \cdot E(\vec{r}_0)\right|^2}{\iint \varepsilon(\vec{r})\left|E(\vec{r})\right|^2 d\vec{r}} \tag{1}$$

Where, n_g is the group index of the mode, n the refractive index at the location of the dipole, $\varepsilon(r)$ is the relative permittivity, **d**-capped is the unit vector along the dipole, and E is the electric field strength of the mode. $P_0 = \omega^4|d_0|^2 /(12\pi\varepsilon_0 c^3)$ is the power radiated by the dipole with dipole strength d_0 in the free-space. If we assume the polarizability, α of the dipole to be a scalar, the dipole strength is proportional to the field at the location of the dipole $d_0 = \alpha E(r_0)$. For simplicity, we neglect the interaction between the particles, change in the refractive index of the cladding caused by the particles and ignore any Stokes shift. It can be shown that the overall efficiency of power coupled back to the waveguide for a given pump power P_{in} is given by the sum of the contribution from each particle lying in the sensing region of the cladding of the waveguide:

$$\frac{P_{wg}}{P_{in}} \equiv \eta = \sum \frac{\pi^2}{n} \left(\frac{\left|E(\vec{r}_0)\right|^2}{\iint \varepsilon_0 \varepsilon(\vec{r})\left|E(\vec{r})\right|^2 d\vec{r}} \frac{\alpha n_g}{\lambda_0}\right)^2 \approx \rho l \int_{sens} ds \frac{\pi^2}{n} \left(\frac{\left|E(\vec{r}_0)\right|^2}{\iint \varepsilon_0 \varepsilon(\vec{r})\left|E(\vec{r})\right|^2 d\vec{r}} \frac{\alpha n_g}{\lambda_0}\right)^2 \tag{2}$$

Where, in the second step, the summation is approximated by the corresponding surface integral in the sensing region taking the product of the density of the particles (ρ) and the length of the waveguide (l). We used COMSOL finite element eigenmode solver to determine the field of the waveguide modes for several waveguide geometries and solve Eq. (2). For simplicity, we neglect material dispersion, pump depletion, and assume $n_g \approx n_{eff}$ as this will have very little impact on our major conclusions.

3. Results and discussions

We assume the polarizability of the molecules to be equal to $\alpha_H = 20 \times 10^{-41}$ C·m²·V⁻¹ which is approximately equal to the mean polarizability of hydrogen molecules [6], concentration of the molecules to be 1 mole/liter and calculate the η for a 1 cm long waveguide. It is emphasized that these representative parameter values we have chosen does not affect the generality of our results because η scales in a simple way with these parameters as per Eq. (2). The new efficiencies for a polarizability α_N, density ρ_N (in moles/lit) and waveguide length l_N (in cm) can be easily calculated using the graphs presented by applying renormalization $(\rho_N l_N) (\alpha_N /\alpha_H)^2$.

Fig. 2 shows the calculated η as a function of the waveguide area A and aspect ratio a for Silicon (Si) and Silicon Nitride (Si_3N_4) waveguides for bulk sensing and surface sensing for a layer of thickness $\lambda_0 /100$ around the waveguide. The maximal efficiency, η_{max} is approximately 5.3×10^{-8} for Si waveguides for bulk sensing, implying that under ideal conditions, for 1mW pump power in the waveguide 53 pW of scattered signal can be collected by the guided mode. The η_{max} for bulk sensing using high index Si waveguides is about 2.4 times larger than that for Si_3N_4 case, while it is about 4.2 times for surface sensing. This implies that surface sensing is more sensitive to index contrast than bulk sensing. The polarizability for fluorescence and Raman scattering can differ by many orders of magnitude from α_H we have used, and a much larger or lower efficiency can be expected as the overall efficiency varies quadratically with the polarizability.

In Fig. 2, we observe strong dependence of η on A and a. For all the sensing scenarios, we observe that the optimal η corresponds to a relatively symmetric waveguide ($0.5 < a < 2$) for both of the quasi-TE and quasi-TM modes. This is rather surprising knowing that, for a given area, a nonsymmetrical waveguide has a larger sensing surface. This means that the effective sensing area is determined predominantly by the modal field properties rather than by the actual sensing area. We also see that the optimal η is less dependent on a for bulk sensing compared to surface sensing. For example, the optimal η for Si (Si_3N_4) waveguides changes by 36% (25%) as we go from $a = 1$ to $a = 5$, while for bulk sensing, the change is only about 19% (13%). Further, the A corresponding to optimal η, for a given a, is higher for surface sensing than for bulk sensing. For instance, for $a=2$, the optimal A for surface sensing is 0.004 λ_0^2 higher than for bulk sensing with Si waveguide while it is 0.048 λ_0^2 higher for Si_3N_4 waveguides. This observation means that a higher optical confinement in the core leads to higher intensity at the waveguide surface and is favored for optimal surface sensing compared to bulk sensing.
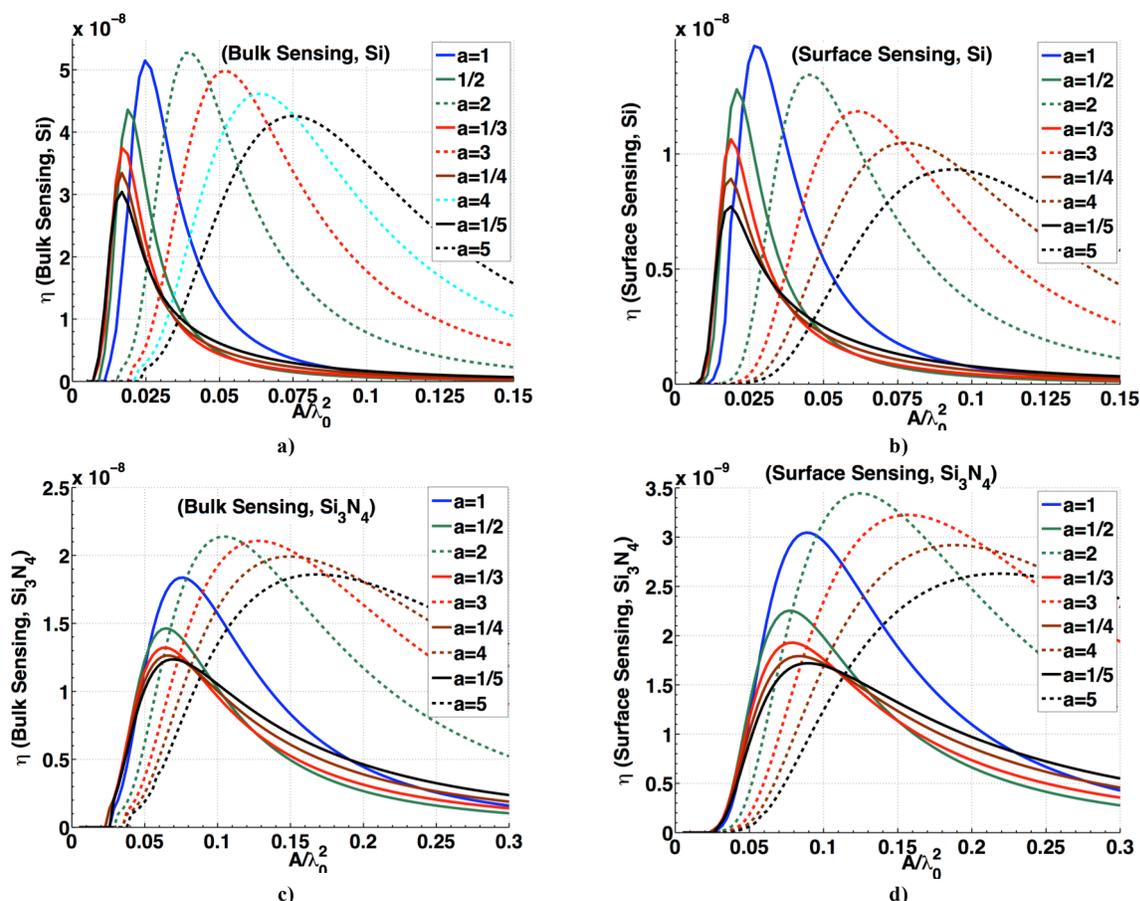
Figure 2: Overall efficiency as function of core area (*A*), normalized to square of free-space wavelength, for several aspect ratios (*a*) for the fundamental quasi-TE modes of a) Si waveguide for bulk sensing, b) Si waveguide for surface sensing, c) Si$_3$N$_4$ waveguide for bulk sensing and d) Si$_3$N$_4$ waveguide for surface sensing. Pump is assumed to be of the same polarization. Note that due to symmetry of the problem, the fundamental quasi-TE mode for *a* =1/*x* is the same as the fundamental quasi-TM mode for *a* = *x*, and for *a* =1 quasi-TE and quasi-TM modes are degenerate.

4. Conclusion

We have calculated the overall efficiency of excitation of molecules and subsequent collection of the emission from the molecules into the fundamental quasi-TE and quasi-TM modes of channel waveguides of several dimensions, for two common sensing scenarios. We have shown that this efficiency is highly dependent on modal properties and optical confinement of the waveguide, which depends on waveguide index and dimensions. We have also shown that there exists an optimal area and an aspect ratio to maximize the overall efficiency for both bulk sensing and surface sensing. For surface sensing, we have demonstrated that a larger core area, thus higher optical confinement is preferred while for bulk sensing, a slightly asymmetrical waveguide is preferred. We have also demonstrated that bulk sensing provides a higher tolerance in terms of waveguide dimensions and core index.

5. References

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