Nanoplasmonic enhancement of Raman signals by a bowtie antenna on a silicon nitride waveguide

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In this paper we numerically investigate the coupling of dipole radiation into an integrated silicon nitride strip waveguide functionalized with a nanoplasmonic bowtie antenna. We show that the antenna can enhance Raman signals by a factor of 10^{10} *and enables efficient coupling of these signals into the fundamental TE-mode of the waveguide. Furthermore the impact of several antenna parameters on the enhancement factor is investigated. Finally we discuss the potential advantages of these structures for on-chip biosensing applications.*

Introduction

Lab-on-a-chip devices, enabling parallel study of multiple analytes, provide an alternative to the existing bulky technologies for spectroscopy and sensing. However, these technologies rely on labeling methods that are intrusive in nature. Either the particles are labeled by means of e.g. fluorescent dyes or the detection surface is functionalized to provide an increased affinity with the particles under study [1, 2]. In this regard, an integrated spectroscopic Raman sensor would enable label-free, high specificity and low-cost sensing platforms. However, Raman signals are inherently very weak and therefore require an additional enhancement mechanism for efficient detection. Surface Enhanced Raman Spectroscopy (SERS) is one such method and is based on the resonant plasmonic behavior of metallic nanoparticles or rough metallic surfaces to enhance Raman signals. Photonic integrated circuits offer the additional advantage of using single mode waveguides for both excitation and collection of Raman signals in a more controlled way. CMOS-compatible photonic integration technologies are particularly relevant in this context since they hold the promise of low cost lab-on-a-chip devices. One can choose between silicon and silicon nitride (Si_3N_4) waveguides depending on the targeted spectral range. It is known that an emission enhancement of dipole radiation can be achieved by means of high-index-contrast (HIC) waveguides and free-space nanoplasmonic antennas [3, 4]. Here we propose a combined approach where a HIC Si_3N_4 strip waveguide is patterned with a nanoplasmonic antenna to achieve enhanced Raman sensing. We consider a dipole located in the vicinity of the nano-antenna, which lies on top of the waveguide, and is excited by the fundamental TE-mode. We restrict ourselves to the TE-case since the TM polarization cannot efficiently excite the configuration under study. It is shown that our combined platform enables a transmission enhancement up to 10^{10} compared to Si_3N_4 waveguides with no nano-antenna on top. The high transmission enhancement combined with the simple excitation and collection approach makes this platform a valuable candidate for single to few molecule SERS.

Numerical Investigation of the Emission Enhancement

In this study we consider a single mode HIC Si_3N_4 strip waveguide ($n = 2.02$, width=600 nm, height=220 nm and λ_0=900 nm) on a SiO_2 substrate ($n = 1.45$) and water cladding ($n = 1.33$) with a gold bowtie antenna on top (Fig. 1(a)). We use the commercial finite element solver COMSOL to study the interaction between the guided mode of the waveguide and a dipole emitter for two cases: a dipole in the gap of the bowtie antenna and a dipole on the same waveguide but without the antenna (Fig. 1(a)). The dipole power coupled to the waveguide mode is denoted by P_{enh} and P_0 for the cases with and without the gold, respectively. The enhancement factor EF is defined as P_{enh}/P_0. In order to test the meshing quality and the different numerical parameters, the total radiated power for a dipole parallel and perpendicular to the core region of a slab waveguide is calculated. An excellent correspondence (average error $\approx$2%) was found between our numerical results and the exact analytical results [5]. The EFs discussed hereafter are therefore expected to have a high accuracy. Since the fundamental TE-mode (polarized along $\mathbf{e}_x$) is used as the excitation field, the dominant and relevant part of the Raman dipole moment is given by $\mathbf{p}_x(\mathbf{r}_0) = \alpha_{xx}\mathbf{E}_x(\mathbf{r}_0)$; α_{xx} is the (1,1) component of the polarizability tensor given by the Kramers-Heisenberg-Dirac formula [6]. Since the highest EFs are expected in the gap of the antenna we only consider dipole positions in this region. Contributions from dipoles that are located outside of the gap region will be much smaller since the EF decays rapidly (the field enhancement region extends only over a few tens of nanometers) In Fig. 1(b) we plot the ratio P_{enh}/P_0 as a function of the ratio $\beta = |\mathbf{E}_{enh}(\mathbf{r}_0)| / |\mathbf{E}_0(\mathbf{r}_0)|$ (each dot corresponds to a different position $\mathbf{r}_0$ of the dipole); $\mathbf{E}_{enh}(\mathbf{r}_0)$ is the enhanced excitation field due to the plasmon resonance and $\mathbf{E}_0(\mathbf{r}_0)$ is the evanescent field of the regular waveguide. The simulation results (red dots) match the fitted β^4 curve (fit based on the β^4 rule of SERS [7]). Since the excitation enhancement scales with β^2 (because the respective dipole moments scale with β), it follows from this figure that the transmitted power by the dipole also scales with β^2. This result shows that there is an efficient coupling of the enhanced emitted power into the fundamental TE-mode of the waveguide (which can be confirmed by a modematching of the TE-mode with the emitted dipole radiation).

The above observations allow us to extract three distinct advantages of using integrated waveguides with a nanoplasmonic structure. Firstly, the plasmons are always excited with the proper polarization to ensure optimal excitation enhancement (a plasmon resonance strongly depends on the orientation of the excitation polarization). Secondly, the nanoplasmonic structure has no detrimental impact on the output power but enables a significant emission enhancement compared to a regular HIC Si_3N_4 waveguide (see Fig. 1(b)). Finally, the emitted signal is coupled efficiently to the fundamental mode of the waveguide. This creates an ideal condition for on-chip spectral analysis of the signal. It is important to note that an absolute value of P_{enh} depends on both the excitation and emission wavelength. For small Stokes shifts, the excitation and emission enhancement factors will be practically equal as the resonance of the combined waveguide-plasmonics system is quite broadband, but for larger shifts the emission enhancement of P_{enh} (and thus the actual output power) will decrease.

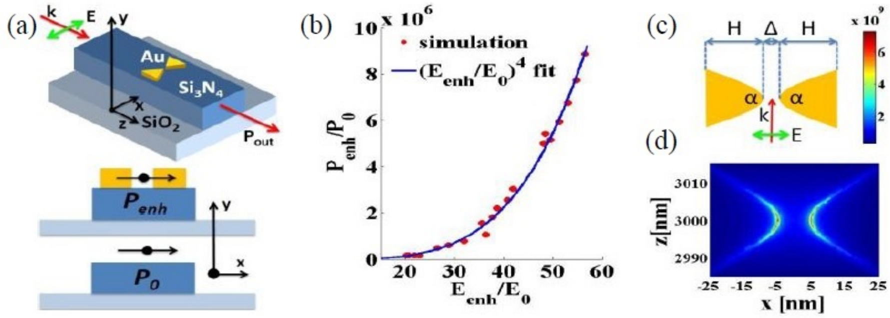

Figure 1: (a) HIC Si_3N_4 strip waveguide with a bowtie antenna; the polarization (green double arrow) and propagation (red arrow) direction of the modal field and the orientation of the radiating dipole are also marked. (b) EF of the Raman power coupled into the guided mode as a function of the field enhancement. (c) Bowtie antenna with dimensions (H, Δ, α). (d) Electric field distribution at the top surface of the gold for $\alpha = 60°$ and Δ=10 nm.

Analysis of the on-chip bowtie antenna

In this section we investigate the impact of the parameters (H, Δ, α) of the bowtie antenna (defined in Fig. 1(c)) to study how we can optimize the excitation and emission of a dipole. The EFs for different geometry parameters are calculated via β^4 since Fig. 1(b) shows that EF scales with β^4. Figure 2(a) gives an example of the field distribution in the gap of the antenna. The strong enhancement at the tips and the steep decay of the EF away from the tips is clearly visible.

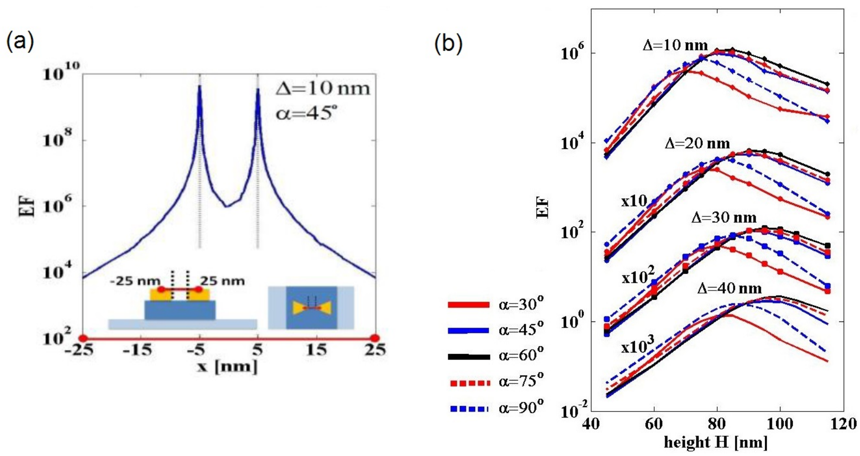

Figure 2: (a) EF at the top surface of the gold; the two inset figures mark the (y,z)-position where the slice (red line) is taken. (b) EF at the center of the bowtie for different (H, Δ, α) parameter combinations.

The simulation results are summarized in Fig. 2(b) where we plot the EF in the center of the gap for different parameter combinations (H, Δ, α). Generally, the optimal height for a given angle is dependent on the gap and for a given gap the optimal height depends on the angle. In the center of the gap, there is a 10^3 order difference for Δ=10 nm and Δ=40 nm and changing H by only 20 nm from the optimal H reduces the EF by 10.

Furthermore, we found that depending on the position of the dipole the EF is maximized for specific values of the (H, Δ, α) triplet. Our study shows that for $\alpha = 30^\circ$ and Δ=10 nm it is possible to obtain transmission enhancements EF up to 10^{10} in a 1 nm region near the tip (the mesh-size near the tip is 1 nm). As such it is clear that adding a properly designed nanoplasmonic structure gives an additional gain up to 10^{10}. This controllable high EF opens the possibility of doing single molecule SERS with our investigated structure. Furthermore our structure can also serve for nanoparticle detection but will be less efficient in the study of larger particles since the EF is large only in a tightly confined (nanosize) region around the metallic nano-antenna. To fabricate these nano-antennas we have explored the Focused Ion Beam (FIB) method but found that the process is not uniform and reproducible for the optimal dimensions from our simulation (see Fig. 2(b)). Therefore an e-beam lithography is currently being explored to produce these structures. The first results show great uniformity and the ability to produce bowties with the desired gap and angle.

Conclusion

In this paper, it is shown that the radiation originating from TE-excited dipoles is efficiently coupled into the fundamental TE-mode of a Si_3N_4 strip waveguide. We also showed that adding a single, well-designed, nanoplasmonic structure has no negative impact on the transmission of the coupled dipole radiation, but is capable of producing Raman scattering enhancements of 10^{10} compared to a simple Si_3N_4 strip waveguide. Furthermore, we investigated the impact of several antenna parameters on the overall performance of the structure and thereby showed that the obtained enhancement can be optimized by tuning the antenna.

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