# Finite element modeling of plasmon based single-photon sources

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***Abstract*—A finite element method (FEM) approach of calculating a single emitter coupled to plasmonic waveguides has been developed. The method consists of a 2D model and a 3D model: (I) In the 2D model, we have calculated the spontaneous emission decay rate of a single emitter into guided plasmonic modes by using the translation symmetry of the waveguides; (II) In the 3D model, we have implemented the FEM calculation to include the radiation modes and the nonradiative contributions by solving the wave equation with a harmonic source terms. The FEM approach is rather flexible, and can handle the plasmonic waveguides with different geometries, as long as only one guided plasmonic mode is predominantly excited.**

## I. Introduction

Substantial efforts have been made to solve the wave equation, especially with arbitrary time dependence. However, only for a few geometries such as spheres and cylinders, one is able to obtain analytical solutions, by the assistance of, e.g., Mie's theory and other modal descriptions. For many other geometries, one has to resort to numerical methods, like finite-difference time-domain (FDTD) method, FEM, or other methods. These numerical methods are indispensable in modern photonics, especially in modeling complex photonic devices. Normally FDTD can model dielectric structures reasonably well, i.e., photonic crystals, however it has severe drawbacks for modeling plasmonic structures due to its typical rectangular grids and the piecewise constant approximation of the fields within grids. And the approximation in dielectric functions of the material in FDTD may give rise to considerable error in broadband calculations. Besides local density of optical states (LDOS) calculations may present additional challenges for FDTD, due to difficulties in accurately transforming $j \cdot E$ from the time to frequency domain. Due to the more advanced discretization strategy for complex geometric structures, and FEM can handle plasmonic structures with strong field localization very well. In many complex photonic environments, it is highly nontrivial to probe the LDOS with acceptable accuracy. In the following, we will report a generally applicable quantitative FEM method to probe LDOS for modeling spontaneous emission (SE) in complex plasmonic structures.

## II. Model

We consider an ideal quantum emitter coupled to a plasmonic waveguide. The excitation energy of the quantum emitter can be dissipated either radiatively or non-radiatively. Radiative relaxation is associated with the emission of a photon, whereas non-radiative relaxation can be various pathways such as coupling to vibrations, resistive heating of the environment, or quenching by other quantum emitters. The resistive heating of the metallic waveguide is the only mechanism of non-radiative relaxation considered in our model. The quantum emitter is positioned in the vicinity of the metallic nanowire, thus there are three channels for the quantum emitter to decay into, i.e., the radiative channel, the plasmonic channel, and the non-radiative channel. The radiative channel accounts for the SE in the form of far field radiation. The plasmonic channel is the excitation of the plasmonic mode, which is guided by the plasmonic waveguide. The non-radiative channel is associated with the resistive heating of the lossy metals, which is due to electron-hole generation inside the metals. The corresponding decay rates are denoted by $\gamma_{rad}$, $\gamma_{pl}$, and $\gamma_{nonrad}$, respectively. The SE $\beta$ factor is defined by $\beta = \frac{\gamma_{pl}}{\gamma_{total}}$, where $\gamma_{total}$ is the sum of the three rates, $\gamma_{total} = \gamma_{rad} + \gamma_{nonrad} + \gamma_{pl}$. The $\beta$ factor gives the probability that the quantum emitter excites a single plasmonic mode.

Due to the invariance along the Z axis, the $Z$ dependence for eigenmodes of an arbitrary (plasmonic) waveguide can be separated, i.e., $\bar{E}(x, y, z) = \bar{E}_\alpha(x, y)e^{-j(\omega t-\beta z)}$. We assign $\alpha = \{p, \beta\}$ to label a guided plasmonic mode, where $\beta$ denotes the propagation constant (the component of the wave vector along the Z-axis), and the index $p$ represents the polarization of the mode. With some algebra, one can determine the normalized decay rate of the emitter oriented along $X$ direction into the plasmonic mode $\alpha$ as given by $\frac{\gamma_{pl}}{\gamma_0} = \frac{3\pi c\varepsilon_0 E_{\alpha_0,X}(\bar{r})E^*_{\alpha_0,X}(\bar{r})}{k_0^2 \int_{A_\infty}(\bar{E}\times\bar{H}^*)\cdot\bar{z}dA}$, where $A_\infty$ denotes integration over the transverse plane, and $E_{\alpha_0,X}$ the $X$ component of electric field for mode $\alpha$. However, it is difficult to calculate the radiation modes in the transverse plane, due to the fact that the field components for the radiation mode in the plane do not vanish no matter how large the modeling domain is. Therefore, we implement a 3D model to include the radiation modes, as well as the nonradiative contributions, by solving the wave equation with a harmonic (time dependent) source term, $[\nabla\times\frac{1}{\mu_r}\nabla\times - k_0^2\varepsilon(\bar{r})]\bar{E}(\bar{r},\omega) - j\omega\mu_0\bar{J}(\omega) = 0$. Concerning the implementation of a FEM calculation, the wave equation needs to be reformulated into its variational form, which enables us to use the standard finite element solution procedures, including discretization and factorization of a sparse matrix. Eventually, the boundary-value problem was solved by utilizing a commercial software package, COMSOL Multiphysics [1]. It is crucial to truncate the computational domain properly. As shown in Fig. 1, we use two techniques for truncating the modeling domain: I) In the X-Y plane, the computation

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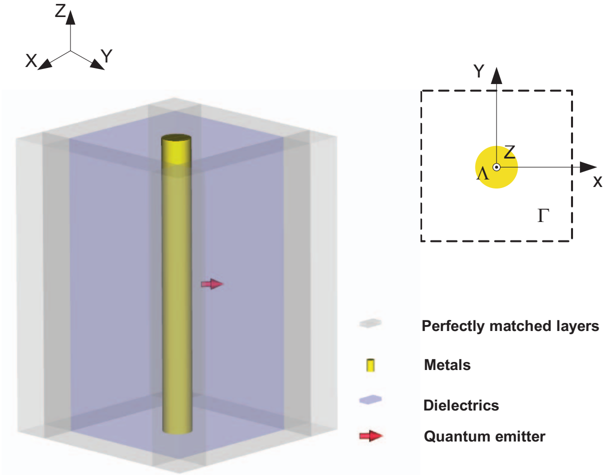


Fig. 1. A single quantum emitter coupled to a metallic nanowire. The grey transparent region represents the perfectly matched layers, the mode matching boundary condition is applied on the top and the bottom of the structure. The quantum emitter is implemented by an electric line current.

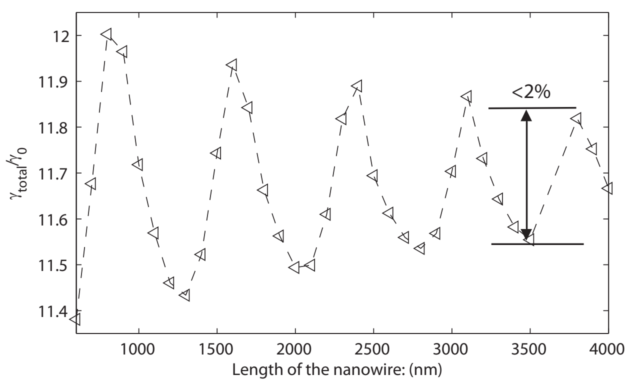


Fig. 2. Length dependence of $\gamma_{total}/\gamma_0$ for the metallic nanowire. The wire radius is 20 nm, the distance to the wire edge is 30 nm.

domain is truncated by the perfectly matched layers. II) Along the Z-axis, the computation domain is terminated by a mode matching boundary condition. There are different options for realizing the mode matching boundary to absorb a single mode, depending on whether the absorbed mode is TE, TM or a hybrid mode. The total decay rate, $\gamma_{total}$, is extracted from the total power dissipation of the current source coupled to the nearby metallic waveguide, $\gamma_{total}/\gamma_0 = P_{total}/P_0$, where $P_{total} = 1/2 \int_V Re(J^* \cdot E_{total})dV$ is the power dissipation of the current source coupled to the metallic waveguide, and $P_0 = 1/2 \int_V Re(J^* \cdot E_0)dV$ is the emitted power by the same current source in vacuum, for further details see Refs. [2,3].

## III. Results and discussions

Essentially the accuracy of $\gamma_{total}/\gamma_0$ depends on the length ($L_0$) of the plasmonic waveguide, i.e., the modeling domain, since radiation modes and other higher order guided modes will be reflected due to a finite $L_0$. We check the validity of the mode matching boundary condition via of $\gamma_{total}/\gamma_0$ for a

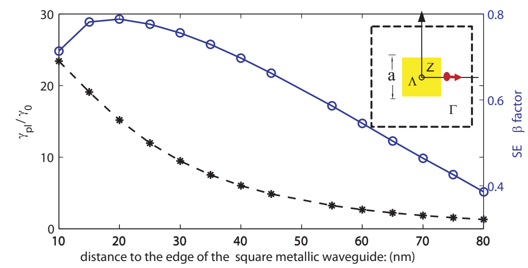


Fig. 3. Distance dependence of the plasmonic decay rates and SE $\beta$ factors for the square plasmonic waveguide.

cylindric nanowire, shown in Fig. 2. The variation in the total decay rate is reduced by increasing $L_0$, and the damped oscillation of the total decay rate with $L_0$ indicates a certain amount of reflection from radiation modes, which is confirmed by the period of the oscillation (equal to the wavelength in a media with $\varepsilon = 2$). The relative error on the computed data is rather small, less than $\pm 1.0\%$ for $L_0$ larger than 1.75 $\mu m$. Using our FEM modeling technique, we studied the coupling of the quantum emitter with a square plasmonic waveguide that are compatible with current lithographic fabrication technology. As shown in the inset in Fig. 3, the emitter is oriented along the $X$ axis, and the distance dependence of the plasmonic decay rates and SE $\beta$ factors is calculated as function of distance from the emitter to the metal surface along the $X$ axis. For the square plasmonic waveguide, though the electric field of the fundamental mode is concentrated around the four corners, one can achieve an efficient coupling between the plasmonic mode and a horizontally oriented quantum emitter. With optimized side length of the waveguide and distance of the emitter to the edge of the waveguide, the $\beta$ factor can reach $80\%$.

## IV. Conclusion

We have developed a robust and flexible FEM modeling technique to study the light emission of a single emitter coupled to plasmon waveguides. Importantly, our FEM approach is also valid for studying light emission in many other structures, like photonic crystal crystal cavities, and optical nanoantennas. We believe our method is useful in the development of efficient optoelectronic devices where the LDOS play a role.

## References

[1] http://www.comsol.com
[2] Y. Chen, T. R. Nielsen, N. Gregersen, P. Lodahl, and J. Mørk, Phys. Rev. B **81**, 125431 (2010).
[3] Y. Chen, N. Gregersen, T. R. Nielsen, J. Mørk, and P. Lodahl, Optics Express, **18**, 12489 (2010).