Optical properties of a waveguide-fed plasmonic nano-array through approximated scattering theory

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***Abstract* — We analyze the optical scattering properties of an array of Au nano-cylinders fabricated upon an ion-exchanged waveguide. The integrated systems is considered for fluoroscopy and Raman spectroscopy. Absorption, scattering and extinction have been calculated through a combination of Finite Difference Time Domain (FDTD) method and scattering theory. While a portion of the excitation signal interacts with the array, the remaining part flows through the waveguide, enabling areas within the simulation box that complicate the calculation through standard procedures. Our analysis includes adjustments and approximations addressing this issue and making full use of computational capabilities of FDTD.**

Keywords — Scattering theory, FDTD, plasmonic nano-array, waveguide, evanescent field.

I. Introduction

Plasmonic nanostructures enable the development of sensors for Biology and Chemistry [1-4], thanks to enhanced fluorescence, Raman scattering and dichroism. In literature, many free-space spectroscopic setups are reported, but it is undoubted that an integrated setup would improve performance and give access to large-scale use [1,2]. In this sense, it would be of interest the development of an enhanced setup consisting of a plasmonic array of nano-cylinders excited through the evanescent field of a waveguide. Such a structure can be arranged within microfluidic channels and alongside fluorescence detectors in order to develop integrated lab-on chips.

In this work, we analyze the scattering parameters of arrays of nano-cylinders fed by the evanescent fields of light propagating through low-index waveguides. This study makes use of Finite Difference Time Domain (FDTD) method and scattering theory [5], accordingly adjusted in order to achieve the most realistic results.

II. Optical Structure and Working Principle

The considered array of nano-cylinders is placed upon an ion-exchanged waveguide (Figure 1). The nano-array and the waveguide are expected to be exposed to an environment rich of water (n≈1.3). The waveguide is a double ion-exchanged one, obtained in a melt of KNO_3 and $AgNO_3$ on a BK7 glass substrate [6-9]. This results in regions within the substrate where the refractive index is slightly higher than in the rest of the sample and where the profile follows a gaussian distribution. This kind of waveguide enables an easy fabrication of nano-arrays through Electron Beam Lithography, since a flat glass surface is a preferential substrate.

The geometrical dimensions of the array are designed in advance to provide the required enhancement. The starting parameters considered in this work are close to others previously adopted [10], namely square array with 250 nm array period of 100 nm diameter and 50 nm thick cylinders.

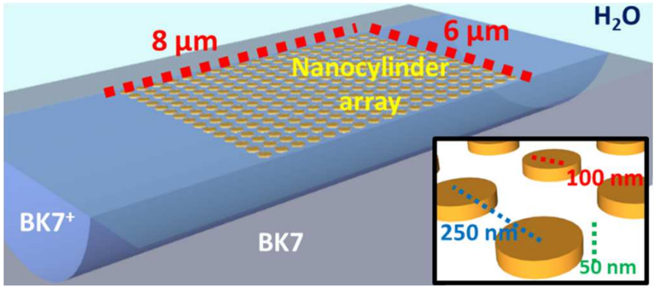

Figure 1: Schematic view of the structure under analysis. The inset shows the details of the nano-array.

III. Scattering Parameter Analysis Formulation

Scattering theory is usually described as in Figure 2a, where the electromagnetic characteristics of an object within a homogeneous and isotropic volume are obtained from E and H fields acquired over the covering surface (monitor-box) [5]. Usually, the source is a plane wave.

In order to extract the scattering parameters, the volume is simulated with and without the scattering objects and the field is obtained from the covering surface. In our specific case, simulations are operated through 3D-FDTD method and the encasing box is cubic. Thus, E_m and H_m are derived from the main simulation, while E_{ref} and H_{ref} from the reference simulation. From the main simulation group, it is possible to directly calculate the absorbed power (W_{abs}) through:

$$Re\left(\frac{1}{2}\oint_S \left(\bar{E}_m \times \bar{H}_m^*\right) d\bar{S}\right) = -W_{abs} \quad (1)$$

whereas, the component of the main simulation related to the scattered field are obtained from the field in the reference simulation box.

$$\bar{E}_m = \bar{E}_{ref} + \bar{E}_s; \quad \bar{H}_m^* = \bar{H}_{ref}^* + \bar{H}_s^* \quad (2)$$

where $\bar{E}_s$ and $\bar{H}_s$ correspond to scattered field's components. Apart from being absorbed, the incident field can be redirected in different directions than the source, thus being scattered away. The sum of scattered and absorbed signals is defined as extinction, which can be computed as:

$$Re\left(\frac{1}{2}\oint_S \left(\bar{E}_{ref} \times \bar{H}_{ref}^*\right) d\bar{S}\right) + Re\left(\frac{1}{2}\oint_S \left(\bar{E}_s \times \bar{H}_s^*\right) d\bar{S}\right) +$$

$$+ Re\left(\frac{1}{2}\oint_S \left(\left(\bar{E}_{ref} \times \bar{H}_s^*\right) + \left(\bar{E}_s \times \bar{H}_{ref}^*\right)\right) d\bar{S}\right) = -W_{abs} \quad (3)$$

In Eq. (3), the first term is expected to be 0 (since the box is empty inside and the source is outside), the second term is the total scattering (W_s) and the third one is the opposite of the extinction, that is:

$$W_{ext} = W_s + W_{abs} \quad (4)$$

In this work, there are various materials inside the box, and the source is the waveguide mode (Figure 2b).

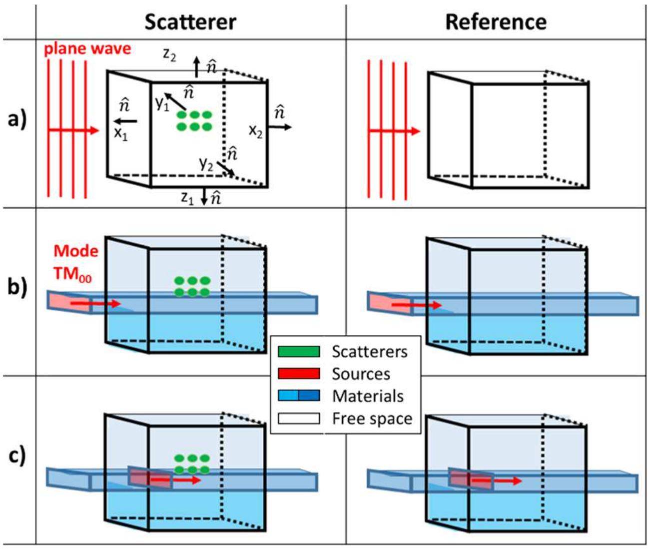

Figure 2: Setup approaches in terms of monitor box and source type: (a) classical configuration, (b) waveguide with source outside the box, (c) waveguide with source inside box.

Part of the waveguide signal is transferred towards the scattering objects, and part of it moves away from the output monitor in the box (x_2 in Figure 2b). In this situation, Eq. (1), (3) and (4) are still perfectly valid, while Eq. (2) is not, since there are intersections between the waveguide and the box where the weak scattered field is mixed with the strong signal flowing through. If those regions are included in the calculation, Eq. (2) would give a misleading amount of scattered field. In order to avoid the ambiguity, two simplifications are adopted. Since FDTD solvers allow considering dipolar and unidirectional sources, the waveguide signal source is supposed to be within the enclosing box, thus making the box itself an active object. In this way, one of the box monitors (x_1 in Figure 2) is impinged almost exclusively by the scattered field. Furthermore, the other intersection, where the output waveguide corresponds to the box monitor, is removed from the calculation. While this assumption conceptually opens the enclosing box, from a numerical perspective it removes unreasonable values in the scattering parameters (see results).

Due to the novel approach with the internal source (W_{source}) within the box, in place of Eq. (1) we have:

$$Re\left(\frac{1}{2}\oint_S \left(\bar{E}_m \times \bar{H}_m^*\right) d\bar{S}\right) = W_{source} - W_{abs} \qquad (5)$$

With the new approximations, relations in Eq. (2) are again numerically valid. If Eq. (2) is introduced into Eq. (5), their combination can again produce Eq. (4), since the first term of the counterpart of Eq. (3) is equal to W_{source}, which simplifies with the right-hand side of the equation.

Finally, it is worth noting that in the 3D-FDTD simulations between input and output waveguide intersections with the box, the former has always more scattered signal than the latter.

IV. Numerical Results

We have implemented the structure in a 3D-FDTD solver and obtained the box field values in both main and reference simulations. The source is at 650 nm wavelength and the boundary conditions are set to Perfectly Matched Layers (PML). Figure 3 shows the results together with the scattering

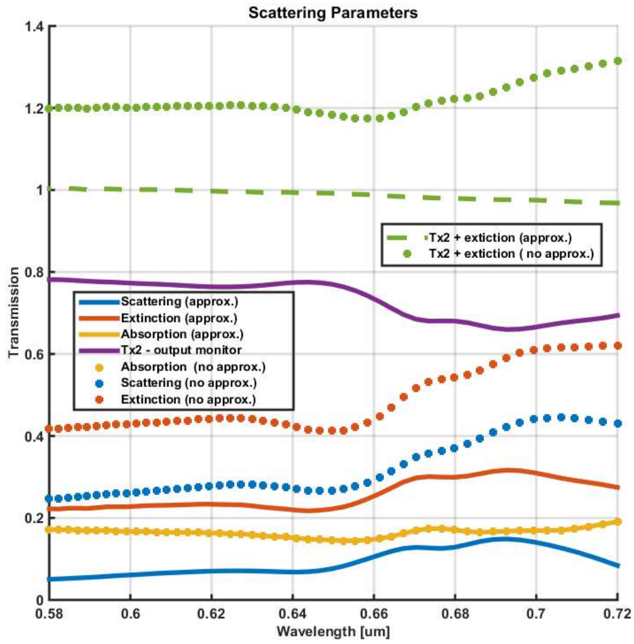

Figure 3: Simulation results after Scattering Theory processing.

parameters in a situation without approximations. As it can be seen, while the absorption values result the same, the scattering field (and thus the extinction) is overestimated in case of no approximation (the residual power added to extinction is higher than 1).

V. Conclusions

A plasmonic array evanescently fed by an optical waveguide has been studied by means of FDTD simulations and scattering theory. The intersection of the waveguide with the simulation box forced us to introduce simplifications on the classical formulation, in order to obtain realistic scattering values. A similar approach can be used in the future to calculate radiation patterns of the scattered field. Overall, the development of practical methods exploiting modern computational tools is needed for the design of integrated optical spectroscopy setups integrating plasmonic nano-arrays capable of enhancing fluorescence, phosphorescence or Raman scattering.

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