Electric Field Distribution of Nanohole Thin Gold Film for Plasmonic Biosensor: Finite Element Method

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***Abstract*—In this paper, we simulate the local electric field distribution and the transmission in 20 nm thin gold films perforated by single sub-wavelength nanoholes on SiO_2 dielectric substrate, immersed in air and illuminated by a perpendicular plane wave. In such nanostructure, intense electric fields are observed secure to the top and bottom nanohole edges under appropriate simulation conditions. Using Finite Element Method (FEM), we simulate the electric field distribution at resonance wavelengths in this nanostructure. More specifically, we show the diameter nanohole effect the plasmonic field enhancement in the edges. Furthermore, we study the effect of the side excitation which plays a key role in the enhancement of this field.**

***Index Terms*—SPR sensor, nanostructure, single nanohole, FEM, side excitation, enhancement electric field**

I. Introduction

It is well known that Surface Plasmon Resonance (SPR) is the collective oscillation of conduction electrons at metal-dielectric interface. The nanostructures supported the SPR have several optical advantages, which open their large application prospects from sensors [1] to photonic devices as biosensors [2], [3]. One of the most common types of nanostructures used in plasmonic biosensors is nanoholes in thin metal films. Moreover, the holes can be used to study aspects like molecules trapped in voids at the nanoscale [4]. The surface plasmon resonance in this subwavelength nanoholes in thin metallic films have been largely studied since the discovery of the Extraordinary Optical Transmission (EOT) phenomenon by Ebbesen, *et al*. 1998 [5]. As array of nanoholes, the isolated nanohole in metallic film exhibited also EOT. This transmission was found dependent on intrinsic properties where the several researches have reported to study the effect of hole diameter [6] on the enhancement of the EOT. As well as the EOT, the distribution of plasmonic field in this nanostructures was wide experimentally and numerically studied [5], [7].

This simulation based study aims to understand the electric field distribution and enhancement in a nanostructure consisting a thin metallic film perforated by a single sub-wavelength hole on dielectric substrate immersed on dielectric surrounding medium. More specifically, the goal is to understand how the geometrical properties such as the nanohole size effect the plasmonic field enhancement. In our study, we find that the localized electric field of the nanohole resonance is mostly concentrated around the top and bottom rims of the holes, more enhancement of this field when the hole become larger. We also consider the degree of the electric field in the top-bottom edges and in the hole-dielectric substrate interface, which are important for the presence of biological molecules in biosensors applications. In addition, the effect of the side excitation on the enhancement of this field is investigated.

The outline of this paper is as follows. In the section "Numerical simulation" we discuss two things: firstly, the geometry of our model and the second one, the different steps allows us to simulate the electric field distribution in this nanostructure. The section "Results and Discussion" is dedicated to the study of an air nanohole in gold thin film deposited on substrate silica (SiO_2): effect of size nanohole and side excitation on the enhancement of plasmonic field, we have here used the geometrical parameters and frequency resonances described by the experimental part study of Rindzevicius, *et al.* [3]. Our conclusions and outlook is given in the section "Conclusions and Outlook".

II. Numerical Simulation

Numerical simulations were performed using Finite Element Method (FEM) COMSOL Multiphysics software v4.4 [8] which has been widely used in the simulation of plasmonic devices. Khoury, *et al*. have demonstrated the validity and the accuracy for plasmonic-nanostructure modeling using COMSOL Multiphysics [9]. We use the RF module to solve 2D model Maxwell's equations for optical field distribution and other optical properties. As shown in the Fig. 1(a), a cross section views (x-y plane) of a nanostructure of Au thin film perforated with circular nanohole placed on SiO_2 film (n=1.5) was surrounded by

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air on one side with a refractive index n=1. Dispersion in the Au film was incorporated for the dielectric function was taken from Palik handbook [10]. Port boundary conditions were applied on the boundaries normal to the incident light, and Perfect Electric Conductor (PEC) boundary conditions were applied in the other directions. The Au film thickness and dielectric substrate were 20nm and 100nm, respectively. The nanohole diameter was varied from 60 to 107nm which is much smaller than the gap wavelength model (300-700nm). An extra fine mesh was used, where the maximum element size was set 4nm for all domains (Fig. 1(b)). The field distribution was simulating as a normalized electric field (V/m). To validate the results of the electric field distribution of our model, we compare with those found in literatures [3].

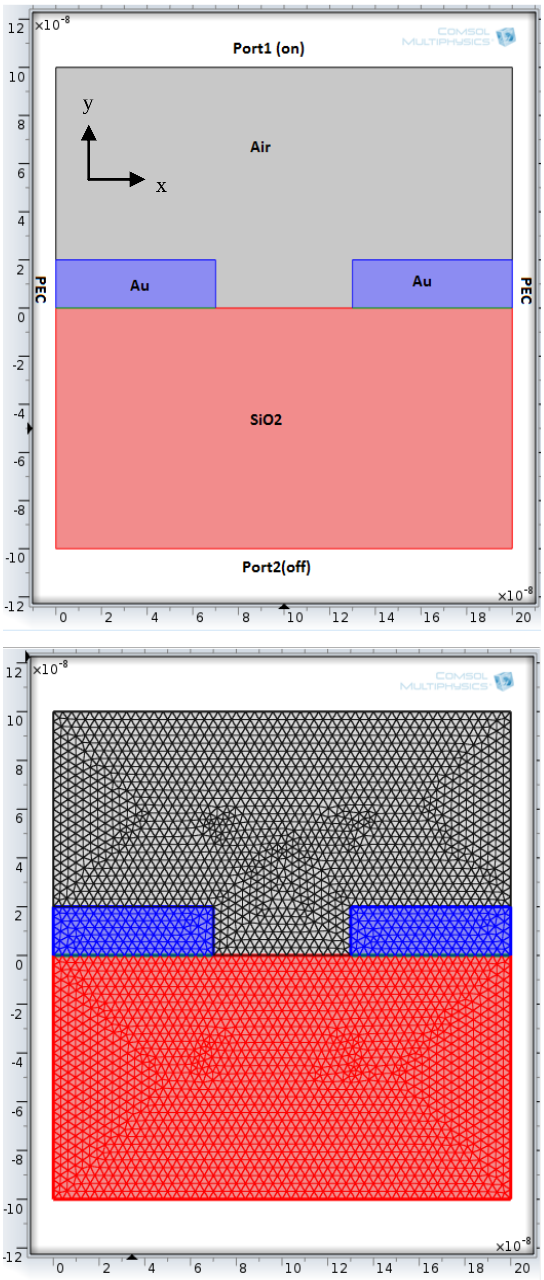


Figure 1. Cross section views (x-y plane) of Au thin film perforated with circular nanohole placed on SiO_2 substrate and surrounded by air on one side, (a) computational domain with the boundary conditions, (b) nanostructure with extra fine mesh.

III. Results and Discussion

A. *Plasmonic Field in Thin Gold Film with Single Nanohole*

Using Finite Element Method (FEM), we simulate the electric field distribution at wavelength resonance of single sub-wavelength nanoholes in 20 nm thin gold film on SiO_2 dielectric substrate, illuminated with a perpendicular plane wave excitation. In Fig. 2(a) the spatial electric field distribution around 60nm nanohole at wavelength resonance 635.9nm is presented. This distribution shows that the higher plasmonic field is secure to the nanohole edges with symmetric field contour. As can be see clearly in Fig. 2(b) the third dimension view (y-z plane) with the maximum electric field spectra of top and bottom left rims of the nanohole as a function the wavelength, the bottom rims of the nanoholes have an intense electric field (5.5 10^5 (v/m)) compared those at top rims(3 10^5 (v/m)), this is due to the difference of refractive index between the substrate/gold thin film and gold thin film/air.

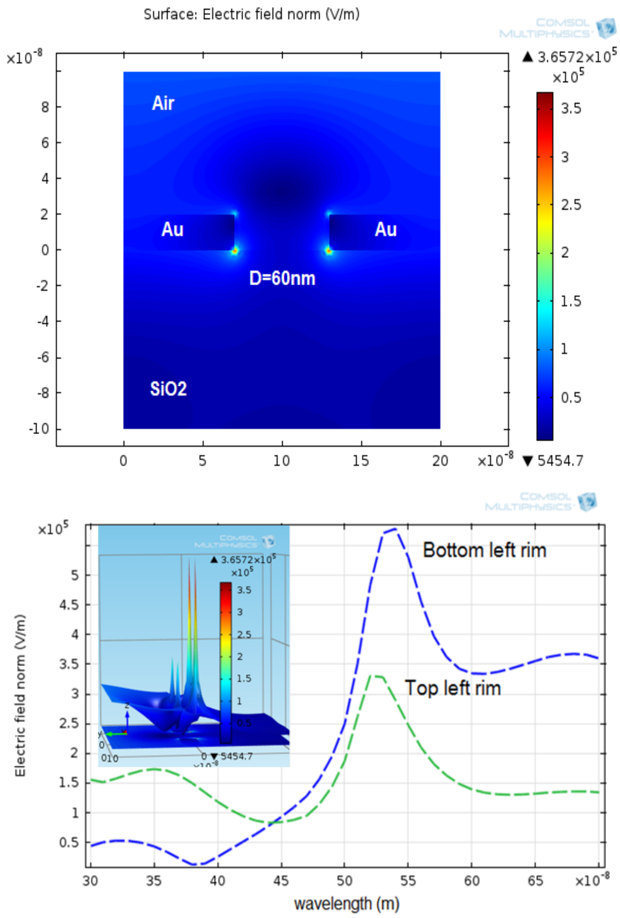


Figure 2. The normalized electric field |*E*| distribution around 60nm hole in a 20nm thick Au film on SiO_2: (a) The cross-sectional views (x-y plane), (b) the maximum electric field spectra of top and bottom left nanohole rims as a function of the wavelength.

B. *Transmission in Terms of Electric Fields*

To illustrate that single nanohole in thin metallic film exhibit extraordinary transmission, using FEM method besed COMSOL Multiphysics software, we simulate zero order transmission. In this softawre, the Radio Frequency (RF) interfaces have a built-in support for S-parameter or scattering parameter calculations. To set up an S-parameter study we use a *Port* boundary feature for each port in the model [8]. In our model presented in Fig. 1, we use two ports with the numbers 1 and 2 and Port 1 is the inport, the software generates the variables S11 and S21. S11 is the S-parameter for the reflected wave and S21 is the S-parameter for the transmitted wave, for more details see S-parameter calculations in the refrence [8].

Fig. 3 shows the calculated transmission spectra or S21 parameter of 60nm hole in gold thin film. As can be seen in this spectra, a peak around 500nm wavelength represent an extratordinary transmission of 70%. When we simulate the electric field distribution at this wavelength resonance (500nm), we notice that there is an enhencemnet in this field from 3.65 10^{-5}v/m (Fig. 2) to 4.47 10^{-5}v/m.

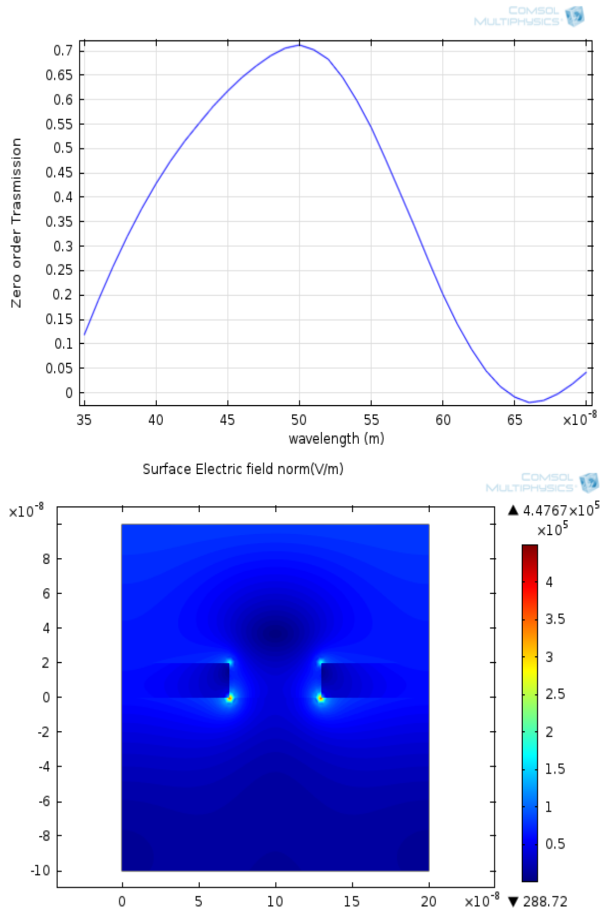


Figure 3. Zero order transmission (a) and normalized electric field |*E*| distribution (b) around 60nm hole in a 20nm thick Au film on SiO_2 at 500nm wavelength.

C. Side Excitation Dependence

In the precedent section, we found that the maximum plasmonic field more concentrated in the bottom edges of the nanohole than top ones. We note that these results are in the case when the nanostructure is excited from the air-gold side. Our focus is on which side of this nanostructure should be illuminated for enhanced the electric field at resonance frequency. Fig. 4 shows cross-sectional view of the electric field distributions (V/m) of 60nm hole in a 20nm thick Au film on SiO_2 for the two cases where the light illuminates the model from the air and from the silica substrate at wavelength 635.9nm. We find that, the plots corresponding SiO_2 side excitation show that the signal in top edges of the nanohole is stronger than that in air side excitation, which means that illuminating from the silica side lead to stronger electric field at air/gold interface. Other than, the electric field at air excitation is correspond surface plasmon resonance wavelength (635.9nm) tended that in the silica side excitation case which have other wavelength resonance.

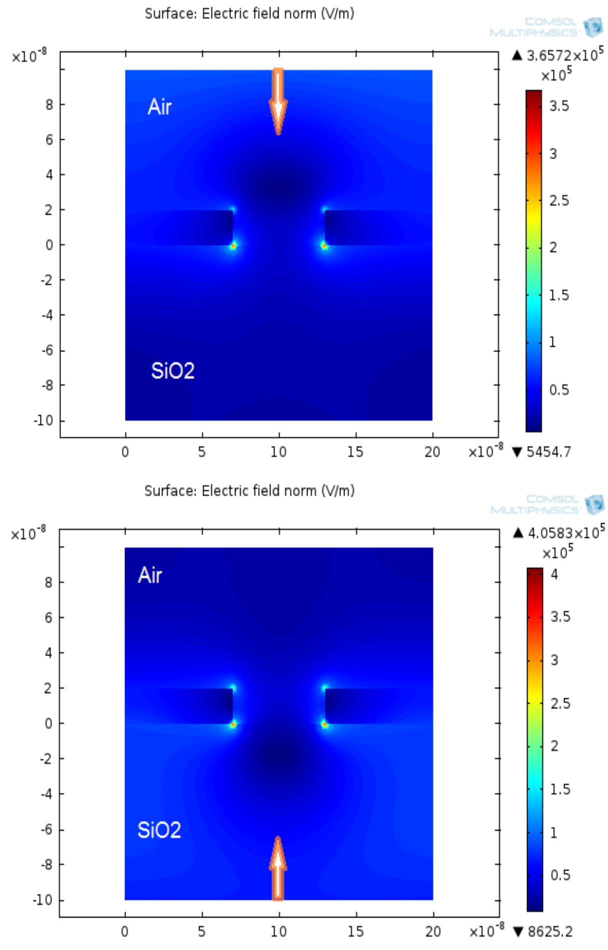


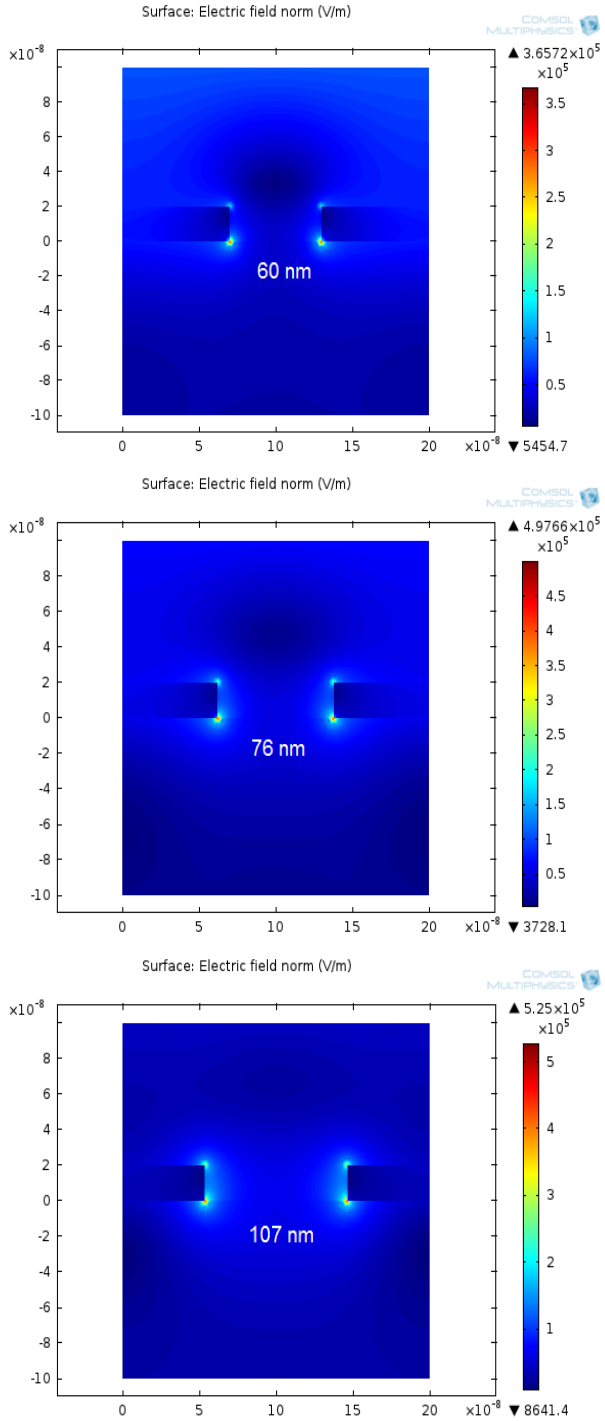
Figure 4. The normalized electric field |*E*| distribution around 60nm hole in a 20nm thick Au film on SiO_2: effect of side excitation (left/ Air side, right/ SiO_2 side).

D. Nanohole Size Dependence

In this section, we study how the size of the nanohole effects the electric field distribution at resonance wavelengths given in Table I bellow. We varied the size of the nanohole from 60nm to 107nm with fixed gold film thickness (20nm) on silica substrate. The cartography of plasmonic field and the variation curve of the maximum value of the electric field are presented in Fig. 5. The results show that, the maximum electric field stays secure to the hole edges although we have changed the size of the nanohole but we can observe a maximum value of this field increases nonlinearly with the diameter of the hole (3.5 for D=60nm and 5 for D=107nm). The maximum plasmonic field falls exponentially with increasing nanohole diameter: E_{max}=-51.05 exp (-D/17.35)+5.16 v. These results are in good agreement with those in literature [3].

TABLE I. VALUE OF WAVELENGTH PLASMONIC RESONANCE CORRESPONDING HOLE DIAMETER TAKEN FROM SCATTERING SPECTRA FROM LITERATURE [3]

Nanohole diameter [nm]	Energy [eV]	Wavelength resonance (λ_{SPR}) [nm]
60	1.95	635.9
76	1.81	685.08
107	1.65	751.52



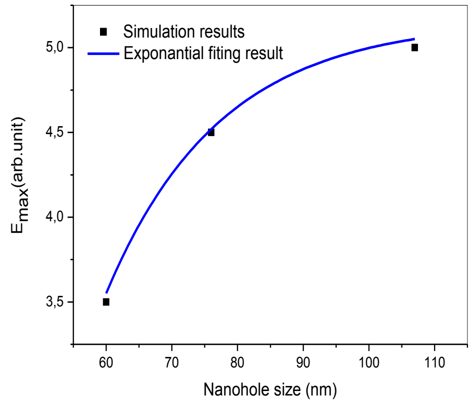


Figure 5. Plasmonic field cartography around 60nm, 76nm and 107nm hole in a 20nm thick Au film on SiO_2. The variation of maximum normalized electric field |*E*| as function of hole diameter.

IV. CONCLUSION

In this paper, we have simulate using COMSOL Multiphysics software based Finite Element Method (FEM) the local electric field distribution in 20 nm thin gold films perforated by single sub-wavelength circular nanohole deposited on SiO_2 dielectric substrate, immersed in air and illuminated by a perpendicular plane wave. Our studies show that the electric field at resonance frequency is concentrated in the rims of the nanohole. In the conditions of simulation, we found that this nanostructure exhibit extraordinary transmission of 70%. The side excitation plays a key role to enhance electric field; the signal of this field at bottom edges was found stronger than that at top ones when the nanostructure is excited from the air side. Furthermore, we find that the size of the nanohole effect plasmonic field enhancement in the edges. The maximum electric field stays secure to the hole edges although and increase exponentially with the diameter of the hole.

The study of the plasmonic field distribution in these nanostructures witch based on nanoholes is an important parameter for biosensors and other nanophotonic applications.

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