16p-D5-5

Simulation of Free-Standing Geometrical Gold Nanoantenna with Variable Post Height for Enhanced Raman Spectroscopy

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1. Introduction

Localized surface plasma is a well-known phenomenon in plasmonics. Due to the interaction with high-frequency electromagnetic fields, electromagnetic coupling could be produced in ordered metal structure array. One of the famous shape arrays is the periodic bowtie antennas, in which two noble metal triangles face tip-to-tip and are separated by a very small gap. Very strong electromagnetic field enhancement can occur between two closely spaced metal triangles, called "nanogap effect [1]." This large enhancement could be used as a tool to enable the single molecule detection via surface-enhanced Raman scattering (SERS). "Free standing" is a new and powerful way to enhance the localized surface plasmon [1]. In this study, we used the finite-difference time-domain (FDTD) method to study the relationship between the surface plasmon resonance and the different geometrical structures.

2. Simulation Setup

The simulation is based on Lumerical Solutions, a commercial FDTD software. In this study, we proposed three geometric structures: bowtie, twin square, and twin hexagonal. The geometric sizes of these structures are defined by their circumscribed circle radius, which is 50 nm in the present study. Two twin geometric structures face tip-to-tip and are separated by an 8 nm nanogap, and consist of a 40 nm thickness gold on an 8 nm thickness chromium adhesion layer, which is located on the top of a silicon post. The silicon post is assumed to be a cylinder with the post height varied from 0 to 300 nm. The self-assembled p-mercaptoaniline (pMA) layer of 0.5 nm thickness is assumed to cover the exposed gold layer. The dielectric properties of Au were taken from Johnson and Christy data [2], Cr and Si were taken from Palik's handbook [3].

3. Results and discussions

Figure 1 is the simulation results of the electromagnetic field enhancement $|E|^2$ as a function of wavelength for different geometric structures. Without the post, the bowtie structure has the highest electromagnetic field enhancement among different geometric structures. When the number of geometric side increases, the electromagnetic field enhancement decreases and blue shift occurs for the resonant wavelength. These resonance peak shifts could be attributed to the change of the charge separation with different geometric structures. The charges on metal structures tend to concentrate at sharp corners and lead to the "lightning rod effect [4]." Compared with the triangles, both the square and hexagonal structures have the smaller charge separation which, in turn, increase the Coulombic restoring force and thus increase the oscillation frequency and shift the resonant peak into the shorter wavelength [4].

The maximum electromagnetic field enhancement $|E|^2$ normalize by the electric field intensity without the Si post as a function of the post height is shown in Figure 2. For all kinds of geometric structures, the optimum silicon post height in our investigation is 100 nm. The maximum electromagnetic field enhancement of bowtie, square, and hexagonal structures with 100 nm post is 9, 5, and 4 times, respectively, of that without the post.

3. Conclusions

In summary, we found that the geometric shape of gold structure plays an important role in determining the plasmon resonance, and blue shift occurs with the increasing number of geometric side because of the smaller charge separation. Furthermore, the numerical results show that the post height of 100 nm is the optimum parameter to produce the strong enhancement for every geometric structure of antenna considered in the present study.

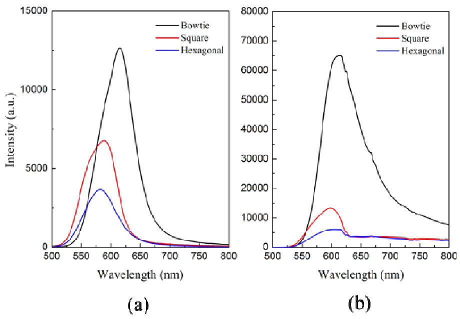

Figure 1. The simulation results of the electric field enhancement $|E|^2$ as a function of wavelength with (a) post = 0 nm (b) post = 200 nm for different geometric structures.

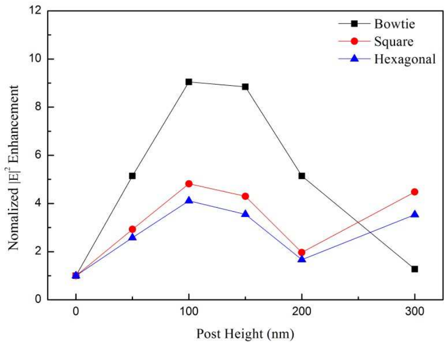

Figure 2. The normalized maximum electric field enhancement $|E|^2$ as a function of post height.

4. Reference

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