Effect of the size and the separation of metal nanodots on the electromagnetic enhancement to surface-enhanced Raman spectroscopy

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INTRODUCTION

Surface-enhanced Raman spectroscopy (SERS) has been intensively researched in the past two decades due to its capability and usefulness as one of the most sensitive detecting tools of high levels of molecular specicity [1], [2], [3]. However, localized surface plasmon resonance (LSPR), which is a major contributor to the electromagnetic (EM) enhancement of SERS, depends on the composition, shape, size, the separation of nanodots, etc [4], their assembly has been studied in detail both experimentally [5] and theoretically. In the latter case, computational electromagnetic methods such as the finite-difference time-domain (FDTD) method and the finite element method (FEM) are often used [6]. Herein, we use the FEM, using an modified version of open-source FEM code, JFEM2D [7], to calculate the electromagnetic enhancement of various assemblies of Au nanodots with SiO_2 coating to predict optimal assemblies for a given incident wavelength. Furthermore, a selected number of $|\mathbf{E}|^4$ at the incident wavelength that give the maximum enhancement for a given geometry will be analyzed to predict "hot spots"[10], which are locations where the maximum EM enhancement occurs.

METHODS

The details on FEM code is described in a code author's article [6]. However, the permittivity values of Au and SiO_2 is modified in accordance with the Mie scattering the correction to nano-scaled metals with coating[8] and with a model dielectric function appropriate to SiO_2 [9], respectively. Figure 1 shows the assembly of interest. Herein, various separations (-5 nm to 10 nm) and radii (60 nm to 120 nm) are used.

DISCUSSION

A sample result is shown in Figure 2. With the separation fixed at 1 nm, assemblies with diameters of 90 nm and 100 nm have maximum EM enhancement when the wavelength of incident field is 813.8 nm. The result also shows that the two Au nanospheres with diameters of 100 nm give higher enhancement than one with diameters of 90 nm at 813 nm. On the other hand, the assembly with diameters of 80 nm give the maximum enhancement at 793 nm, which is a little bit lower than that from assemblies with larger diameters. For the assembly, the contour plot of $|\mathbf{E}|^4$ at 793 nm is plotted in log scale in Figure 3. It shows that the "hot spots" (geometrical locations with the highest enhancement) for the assembly are located between two Au nanospheres.

CONCLUSION

The effect of size and placement of Au nanospheres on the EM enhancement of SERS was studied. The application of these results to quantify the SERS enhancements effects observed for cylindrical dielectrics coated with Au nanodots will be illustrated.

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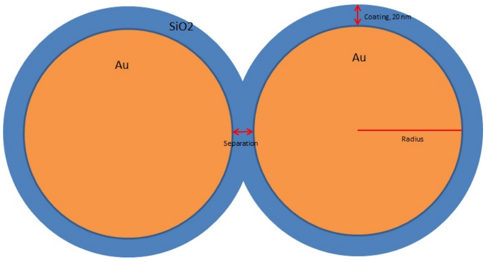

Fig. 1. Assembly of interest. Two gold nano spheres with SiO_2 coating are given

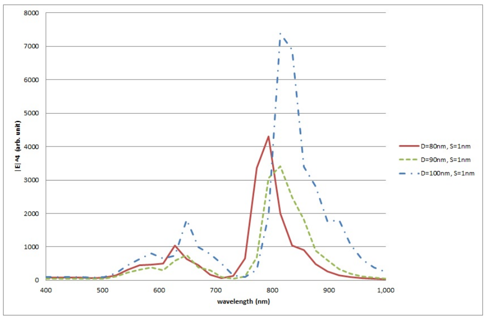

Fig. 2. Maximum electromagnetic enhancements ($|\mathbf{E}|^4$) for nanospheres of 80, 90, 100nm with separations of 1 nm

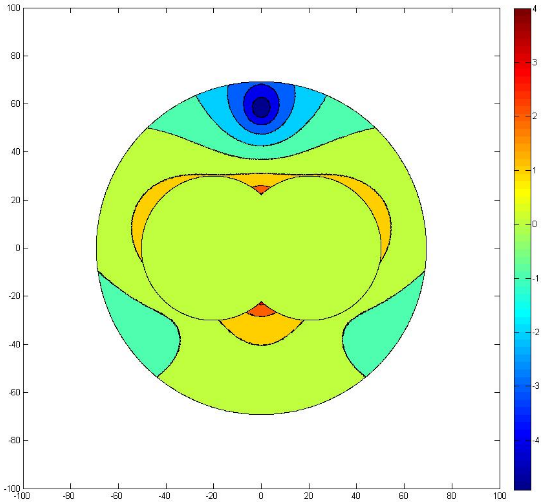

Fig. 3. Contour plot of $|\mathbf{E}|^4$ at the incident wavelength of 793 nm for the assembly with diameter of 80 nm and separation of 1 nm