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Research Paper

Numerical Simulation of Near-Field Enhancement in Silver Nanoparticles

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ABSTRACT

The presented work has simulated and investigated the electromagnetic field enhancement in silver nanoparticle. The electric-field enhancement (EF) in silver monomer and silver dimer is calculated using Finite- Element-Method (FEM). The size of the nanoparticle is tuned to optimize the overall electric field enhancement at two different excitation wavelengths (500 nm and 600 nm). The formation of hot-spot region in the Ag dimer was investigated and analyzed. The simulated results showed that silver-based nanoparticles are efficient plasmonic candidates for Surface enhanced Raman spectroscopic applications.

1. Introduction

Noble metal nanoparticles are promising candidates for all plasmonic applications due to its unique optical properties known as localized surface plasmonic resonance (LSPR) [1-5]. If the nanoparticle size is negligible compared to wavelength of excitation, the dipolar mode will play a dominant role in resonance phenomenon. At a unique frequency, known as localized surface plasmon frequency, the incident electric field differs from applied by a field enhancement factor (EF)[6]. The field enhancement factor, in general, can be tuned to any extent by tuning the size, shape, type of metal and the host matrix. Thus, all-Plasmonic applications can be realized by suitably controlling the material properties.

It can be seen that, the LSPR in metal nanoparticle results in an enhancement in near electric field i.e., the growth of electric field at the vicinity of the nanoparticle surface. Consequently, when two nanoparticles come closer to form Ag dimer there exist region of intense electric field known as the region of hot spot[7-9]. The formation of hotspots is essential for Surface enhanced Raman Spectroscopic (SERS) applications. In which a weak Raman signal from an analyte molecule is strongly amplified at the vicinity of hotspot region. The strength of hotspot can be optimized by suitably controlling the size of the nanoparticles and the separation between them.

Thus, highly desirable in engineering of plasmonic nanostructure for SERS applications [10]. In this context the design of the nanoparticle structure and the optimization of material parameters for optimal plasmonic performance need a special attention. The presented work, employs a Finite Element Method (FEM)[11], a numerical technique to design and the optimization of near field enhancement in silver-based nano-particles at two different excitation wavelengths; i.e. the excitation at 500nm and 600 nm respectively.

2. Numerical Methodology

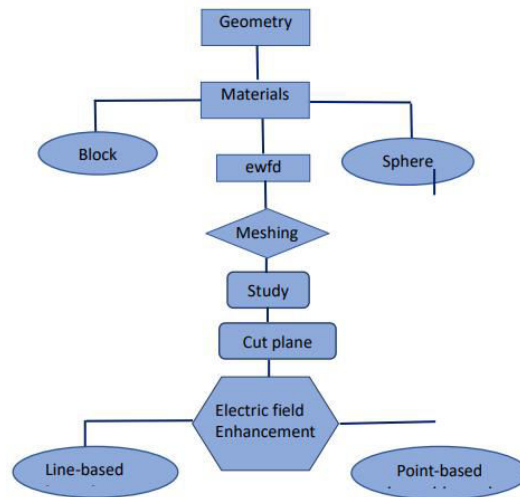
For numerical simulation, COMSOL software (version 6), based on the FEM has been implemented. The important steps involved in the workflow of this COMSOL Multiphysics are given as follows

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The work flow in COMSOL Multiphysics consists of selection of specific geometry, assignment of materials and definition of finite mesh for the chosen geometry. Once the geometry is built a perfectly matched layer (PML) is added to the surroundings; the role of the PML layer is to act as a boundary to absorb the reflected electromagnetic radiation. In general, the electromagnetic waves will get absorbed by PML layer and does not allow it to reflect back to the domain of interest. Meshing plays a very important role in the accuracy and efficiency of FEM simulations, which involves the breakdown of a complex or larger entity into a smaller and finer element called discretization of elements. Due to meshing one can solve any equations using FEM more efficiently [12], [13].

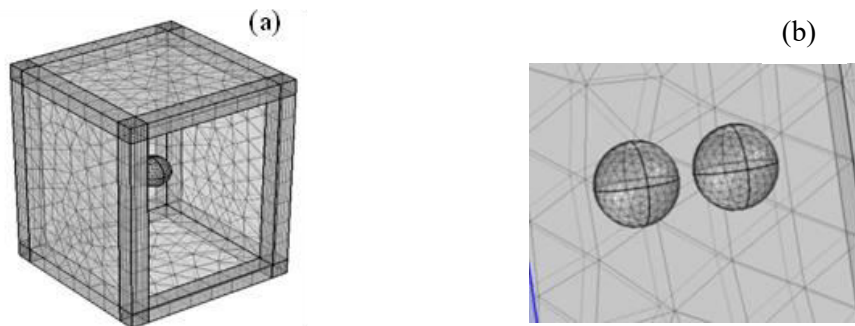


Fig 1: Meshing of (a)Ag monomer with PML and (b) Ag dimer

3. Results and Discussion

Three-dimensional finite element method (FEM) has been utilized to calculate the electric field enhancement in silver nanoparticle configuration such as Ag monomer as well as in Ag dimer. The goal is to optimize the near field enhancement by tuning the material parameter such as the radius nanoparticle for different excitation wave length. Firstly, the calculations are performed for single nanoparticle, which is immersed in a water medium. The excitation parameters are 500nm laser wavelength having an electric field strength of 1 V/cm.

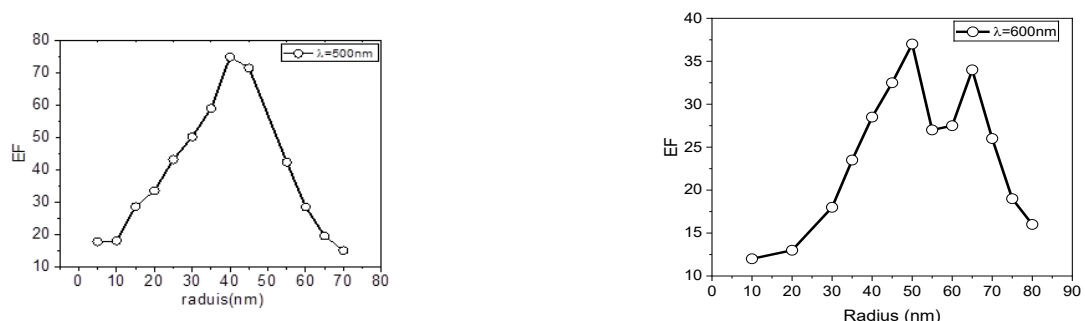


Fig 2: Electric field enhancement (EF) calculated as function of radius of the Ag nano-particle for 500nm (left) and 600nm(right) respectively.

Figure 2 depicts the variation of electric field enhancement calculated as a function of the radius of the nanoparticle. The maximum enhancement is obtained for radius of 35 nm. When nanoparticle radius below 35nm, the dipolar absorption dominates over the scattering while it is reversed in case of larger nanoparticle. For smaller radius of nanoparticle (<35nm) the electric field enhancement is found to be decreased due to the dominance of absorption whereas for the larger radius of the nanoparticle (>35nm), the electric field enhancement reduces due to the increase in scattering

mechanism. Thus, less than 500 nm excitation the optimal radius for field enhancement is 35 nm, in which between the absorption and scattering mechanism balance each other [3], [4].

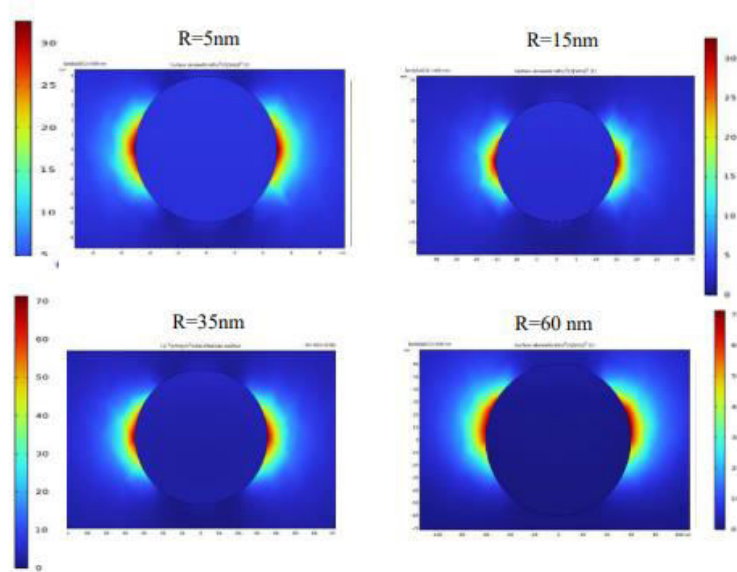


Fig 3. Represents the electric field contour calculated for a single silver (Ag) nanoparticle.

Figure 3 shows the electric field contour calculated as a function of radius of the nanoparticle for excitation wavelength 500 nm. Simulations clearly depict the growth of electric field at the surface of the nanoparticle and it decreases rapidly towards the volume of the nanoparticle.

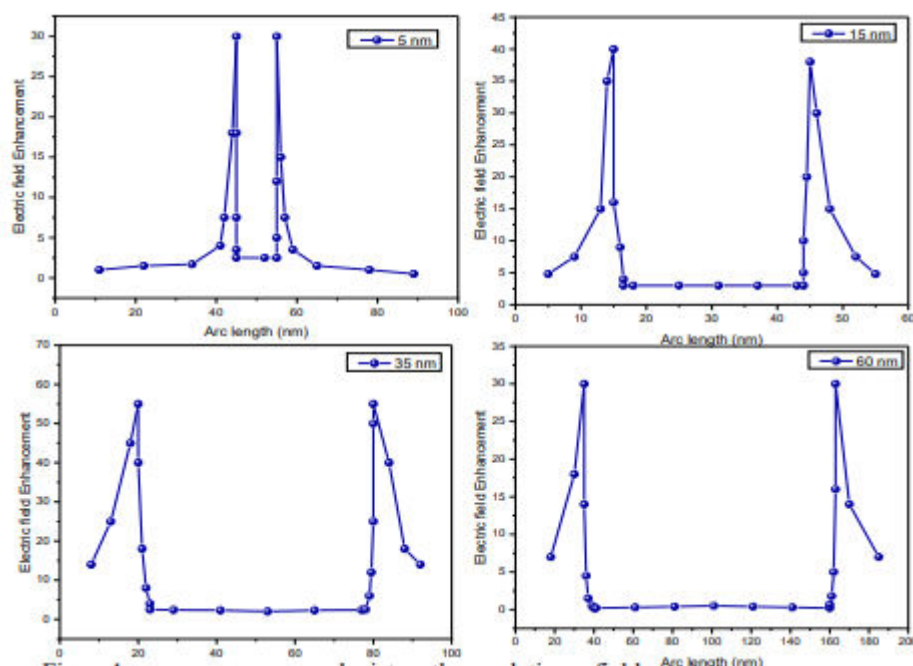


Fig 4 .depicts the relative field enhancement calculated as the function of arc length of nanoparticle at 500 nm excitation wavelength.

Figure 4 denotes the relative electric field enhancement calculated as a function of the arc length of the spherical nanoparticle for the radii 5nm, 15nm, 30 nm and 60 nm respectively. The value of field enhancement is found to be 60 for nanoparticle radius of 35nm whereas the value of the field factor reduces to 20 for 5nm radius at 500nm excitation. Upon selecting the excitation wavelength at 600 nm (~which is far away from LSPR of the Ag nanoparticle) the field enhancement is found to be maximum for radius of 45 nm. Under 600nm excitation, for 45 nm radius, the absorption efficiency effectively balances the scattering efficiency. The simulations are extended to calculate the electric field enhancement in Ag nano-dimers. The dimer configuration shows the formation of hotspot region due to the coupling of dipolar excitation at the Ag nanoparticle and the corresponding electric field enhancement factor is of three orders of magnitude larger than that of Ag monomer configuration. Hence, such a hotspot region in a dimer configuration has the potential usage for the applications such as SERS and SEF. For Ag dimer simulation the chosen parameters are as follows : the radius of 35nm with a dimer gap of 2nm under 500nm excitation as shown in figure 5.

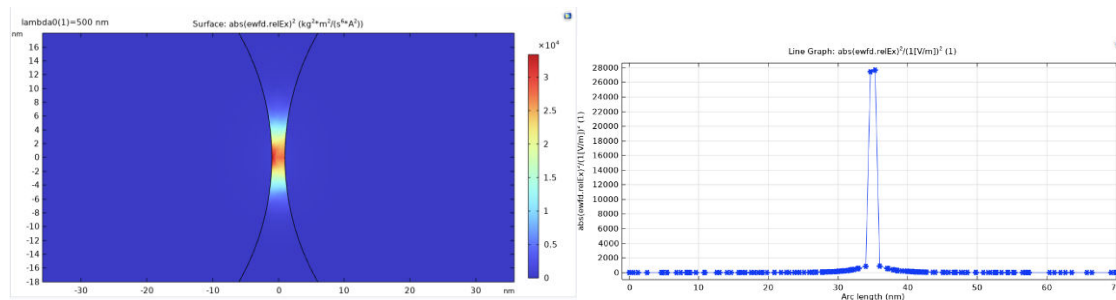


Fig 5. Represents the electric field contour calculated for a Ag dimer and the plot shows the field enhancement calculated as the function of arc length of nanoparticle for the radius of 35nm at 500 nm excitation wavelength.

4. Conclusions

In the presented computational study, COMSOL software based on the finite element method were utilized to calculate the theoretical electric field enhancement in Ag nanoparticle at two excitation wavelengths. Exciting the nanoparticle with 500 nm wavelength shown a maximum electric field enhancement at nanoparticle radius of 35 nm while shifting the excitation wavelength to 600 nm reduces the field enhancement to considerable extend. For Ag dimer configuration, the large growth in electric field enhancement due to the coupling between the dipolar modes is observed. The presented study provides a general understanding of electric field enhancement in Ag based plasmonic nanoparticles.

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Conflicts of interest: The author declares no conflicts of interest.

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