Investigation of plasmonic effects on the metal nanoparticle arrays for biosensor applications

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Abstract. Surface plasmon resonance (SPR) on the near field intensity of a two-dimensional (2-D) periodic arrays of bowtie-shape metal nanoparticle (MNP) pairs using the 3-D finite element method (FEM) for biosensor applications are investigated. The peak resonance wavelength can be shifted to red as the filling core media in bowtie-shape MNP pairs have been changed. The tunable and highly sensitive SPR modes are observed due to the hybridization SPR effects. Simulation results show that the peak resonance wavelength ($\lambda_{\text{res}}$) can be spread in the full wavelength range of 300-1600 nm when the tip edges and different filling media in structure are taken into account. The highly sensitive optical performances give us a qualitative idea of the geometrical and material properties of the periodic array of bowtie-shape MNP pairs on SPRs that can be as a promising candidate for plasmonic biosensor applications.

1. Introduction

The surface plasmon resonances (SPRs) arising from noble metal nanoparticles (MNPs) (e.g., gold or silver) are highly attractive due to their diverse application in nanophotonic field [1-7]. These MNPs mainly can be applied to sense the biological nanoparticles [1]. Tunable peak resonance wavelength ($\lambda_{\text{res}}$) can be manipulated by dimensions, aspects and the surrounding media of MNPs [2]. Recently, several numerical and experimental works on single or a pair of MNPs has been investigated and the tunable plasmonic effects can be found in the scattering and absorption spectra [3-5]. Dramatic SPR modes are excited at the extremity of the finite chain of MNPs [6]. These results correspond to the surface enhanced Raman scattering by molecules adsorbed on MNPs, which can be applied in plasmonic biosensors [7].

The periodic array of bowtie-shape MNP pairs can be served as plasmonic orientation sensors due to its strong gap enhancement capabilities. Several studies regarding on single or dimer rod-shape MNPs have already demonstrated the rich variety of optical properties [3-5], but rarely deal with the periodic array of bowtie-shape MNP pairs. The optical properties of the periodic array of bowtie-shape MNP pairs with different filling media and structural aspects are still not very clearly understood. This periodic array of bowtie-shape MNP pairs could open up the more challenge to explore the plasmonic effect of the dipolar and cavity plasmon on the near field intensity spectra. This includes a closer study of the influences of the distribution of electric field (E-field) intensities and charge density distributions on the periodic array of bowtie-shape MNP pairs. In this paper, a design strategy to obtain tunable mode field enhancement in the nanoscale focal spots of a 2-D periodic array of bowtie-shape MNP pairs is investigated. The unit cell of the proposed structure is composed of a pair of identical bowtie-shape silver (Ag) with filling dielectric constants ($\varepsilon$) in the structural arms. The
influence of its structural and material parameters on the MNP resonance conditions will be examined and compared to their solid case of counterpart. Numerical simulations are performed by using the 3-D finite element method (FEM) of Maxwell’s equations. It would be desirable to tune the $\lambda_{res}$ of these SPR modes to allow the near field intensity spectra to be broadened without changing the outer dimension of MNPs, but it allows for the change of filling media and tip edges in the structures.

2. Simulation method
In the numerical simulations, Ag MNPs described by permittivity data in Ref. [8] was considered. The simulation models are shown in Figure 1(a)-(c), i.e., (a) truncate view of a 2-D periodic array of bowtie-shape MNP pairs, (b) a unit cell of a solid bowtie-shape MNP pair and (c) a unit cell of a dielectric-hole (DH) bowtie-shape MNP pair. The parameters used in the simulations are listed in the inset of Figure 1. Referring to Figure 1, $x$, $P$ and $g$ are the length of a bowtie-shape MNP pair, period length ($P_c$ along $x$-axis and $P$ along $y$-axis) and gap distance between two adjacent bowtie-shape MNPs, respectively. For duplicating the periodic array structures, the 2-D arrays are obtained from the unit cell by using periodic boundary conditions (PBC) along the $x$- and $y$-axes and the scattering boundary conditions along the electromagnetic (EM) wave propagation direction [7], i.e. the $z$-axis. The incident EM waves were performed by fixing at $|E_0|=1$V/m and the simulation models are illuminated by normal incidence EM wave with $x$-polarization (or transverse polarization).

3. Results and discussion
Figure 2 shows the near field intensity spectra (Figure 2(a)-(c), E-field), electric field (E-field) intensity distribution (Figure 2 (d)) and surface charge densities (Figure 2 (e)-(f)) of a solid bowtie-shape MNP case and DH bowtie-shape MNP cases with various core media ($\varepsilon$) and shell thickness ($t$). The $\lambda_{res}$ of the transverse modes are changed upon varying the core dielectric constant ($1<\varepsilon<5$, in step of 1). The simulated near field intensity spectra obtained at various $\varepsilon$ show a red shift of $\lambda_{res}$ position with the increasing of $\varepsilon$ [7], which can be used for the biosensor applications. The sensitivity is related to the spectral position of the MNP resonance and the hybridization of the SPR and core medium effects in cavities [9, 10]. The E-field in MNP gap reaches a peak value at which the Fabry-Perot resonance condition is satisfied [11]. By tailoring the E-field intensity in the MNP gap and core regions, the sensitive operations can be produced from the MNP gaps, making the DH suitable for probing a small number of atoms or molecules localized in the gap and core regions [7, 12, 13]. This finding will be beneficial to the application for single molecule analysis [14].

Next, we use the shell thickness ($5<t<15$ nm), as a tuning parameter and an evident difference on optical properties is observed among the two cases. It can be observed that the resonance peaks in $t=5$ nm case occur in the wavelength range of 350–550 nm and 675–860 nm at different filling $\varepsilon$ in DHs, and the $\lambda_{res}$ redshift and decrease as the filling $\varepsilon$ in DHs is increased. For the case of $t=10$ nm (Figure 2(b)), the resonance peaks are shrunk in the wavelength range of 375–450 nm and 550–690 nm at

![Figure 1. Schematic plot of simulation models.](image)
different filling $\varepsilon$ in DHs, and the $\lambda_{\text{res}}$ redshift and decrease as the filling $\varepsilon$ in DHs is increased. It is worthy to note that there are two resonances in bowtie-shape MNP DH cases, i.e., the first one $\lambda_{\text{res}}$ is due to high frequency (short wavelength) oscillation between MNP and incident light [7] and the second one results from the interaction of the two identical MNPs (corresponding to structure resonance) and core medium effect (corresponding to cavity resonances) [15]. In addition, it can be found that when MNP shell thickness is thicker ($t=15$ nm, Figure 2(c)), the $\lambda_{\text{res}}$ will be shrunk to a shorter wavelength range and their performance is similar to the solid bowtie-shape MNP case, which is due to the shell thickness approaching the bulk Ag mean free path.

![Figure 2](image-url)

Figure 2. (a)-(c) Near field intensity spectra, (d) E-field intensity distribution and (e)-(f) surface charge densities of a solid bowtie-shape MNP case and the bowtie-shape DH MNP cases with various filling media ($\varepsilon$) and shell thickness ($t$).
Likewise, regarding the E-field intensity distribution (Figure 2 (d)), the corresponding charge distributions in two cases are depicted in Figure 2(e)-(h), respectively. The charge distributions on the edge surface of MNPs obtained from the DH cases are larger than those of the solid one. This is because of the hybridization of the void plasmon and liner localized SPR effects [16], namely, both the SPR and cavity modes can be found in the DH cases. It is evident that the local field enhancement can be found on the inner and outer surface of the bowtie-shape MNP DH cases (Figure 2 (d)).

Finally, the E-field enhancement arising from the tip edge will be included in the simulations and the width of tip edge length (w) of 10 nm is considered. The simulation model is depicted in the inset of Figure 3. Figure 3 suggests that we have found that the combination of tip edges and the change of filling ε can significantly tune the λ_{res} in the considered bowtie-shape MNP DH cases while the outer dimension of MNP structure is kept constant. The near field intensity distributions on the inner and outer surface of MNPs show a field enhancement on the surface of tip edges (see the inset of Figure 3). It is evident from Figure 3 that the λ_{res} can be extended in a full wavelength range of 300-1600 nm and this phenomenon cannot be found in the solid case and the bowtie-shape MNP DH cases without tip edges (Figure 2(a)-(e)). It can be attributed to the combination of coupling effects among the incident EM waves, gap regions, core media (ε) and MNP tip edges connecting them is preferable for the positive-negative charge pair excitation on the surface of MNPs [17]. Besides, the coupling effect between two tip apices of MNPs results in edge enhancement in the gap region [18, 19]. Such gap enhancement and environmental sensitivity of the plasmons holds great potential for monitoring local environmental changes during chemical or biological processes. These results may have significant implications for the optimal application of the plasmonic MNP arrays based biosensor configurations.

**Figure 3.** Near field intensity spectra arising from the combination of tip edge and filling core media in the solid bow-tie MNP case and the DH bowtie-shape MNP cases.

4. Conclusion
In conclusion, the purpose of this study is to understand and develop more efficient MNPs for plasmonic biosensor applications. In this paper, the periodic array of bowtie-shape DH MNP pairs which unit cell is composed of two identical nanometals with the filling media and tip edges by using the 3D FEM have been investigated. The tunable and sensitive SPR modes are observed. Simulation results show that the resonant wavelength of the proposed structure can be dramatically tuned over a broad spectral by considering the filling media and introducing the tip edges in the structures simultaneously. This phenomenon cannot be found in the cases without the core-shell and tip edges in structures. The proposed structure promises applications in single molecule surface enhanced Raman spectroscopy (SERS) and plasmonic biosensor owing to its high local field enhancements and large
scale manufacturability. In the near future, further experimental works related to the proposed structure will be performed to demonstrate the results in this work more convincing.

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