Optical Properties of Modified Nanorod Particles for Biomedical Sensing

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***Abstract*— In this contribution we propose a computational investigation of modified gold nanorod particles operating in the Visible and Near Infrared frequency regime. The modified particles consist in a core/shell structure (SiO_2/Au) embedded in a dielectric environment. The nanoparticles optical properties in terms of resonant behavior and near electric field distribution are numerically evaluated. Then, the sensitivity performance of the structure is analyzed for biomedical applications. The obtained results are compared to the other ones of the classical rod particles.**

***Index Terms*—nanoparticles, nanostructures, nanoscale devices, nanophotonics.**

I. Introduction

Localized Surface Plasmon Resonance (LSPR) excitation arises from the interaction between the electromagnetic field in the Visibile (VIS) and Near Infrared frequency Regime (NIR) with small metal particles. The incident electromagnetic field induces the electrons collectively oscillation of the metallic nanoparticles. The resonant condition of the electron motion is related to the size, shape, particle electromagnetic properties and to the refractive index of the surrounding dielectric environment [1].

The unusual optical properties derive from the strong local electromagnetic field enhancement in the neighborhood of the structure under this excitation. Therefore, such structures are very sensitive to changes in the refractive index of the surrounding dielectric medium. These characteristics make metallic nanoparticles suitable for several biomedical applications [2,3].

Nowadays many researches have focalized the attention on the optical properties of nanorod particles. In particular, it is well known that this particle exhibits both longitudinal and transverse plasmon modes [4]. The electromagnetic excitation of each mode depends on the orientation of the particle respect to the electric filed oscillation axis as well as the geometrical length distribution of each axis. Moreover the linear dependency of the resonant peak position of each mode respect to the geometrical dimension of the particle has been reported [5].

In this contest, we propose modified nanorod particles consisting of a core/shell structure (SiO_2/Au) embedded in a dielectric environment. These particles allows to add another degree of freedom (shell thickness) in the design of the optical response compared to the classical one.

By varying the particle shell thickness the sensitivity performance are evaluated. A sensitivity comparison between classical rod particle and modified one with the same volume is shown.

II. Model of Modified Nanorod Particles

The proposed geometry consists in a rod-shaped particle with SiO_2 core and Au thin shell (Fig. 1). To estimate the optical properties of such structure the finite integration commercial code CST Studio Suite has been used. In the simulations we have used a time-domain method based on finite integration technique (FIT). In particular, the structure is discretized using hexagonal mesh. The permittivity value for the SiO_2 core was taken to be $1.44+0i$ at all wavelengths. For gold shell the experimental values of complex permittivity dispersion as reported in [6] have been used. The surrounding dielectric medium is considered to be vacuum.

To evaluate both longitudinal and transverse plasmon modes we have employed two type of excitation. In both of them the structure is illuminated by a plane wave with the propagation vector **k** perpendicular to the longitudinal/transverse axis. The difference consists in the electric filed oscillation axis as depicted in Fig. 1.

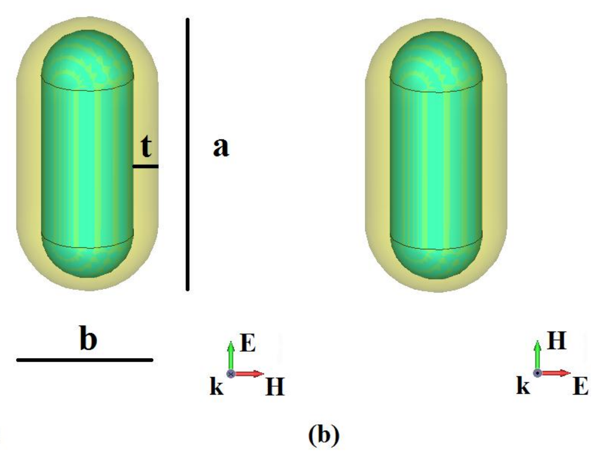

Fig. 1. Core/shell nanorod particles: (a) longitudinal plasmon mode excitation, (b) transverse plasmon mode excitation. Geometrical parameters: $a=80$; $b=40$; $5<t<11$. All dimensions are expressed in nm.

If the plane wave impinges on the particle with an inclined incident angle both longitudinal and transverse plasmon modes can be simultaneously excited.

In Fig. 2 the extinction cross-section spectra for different values of the thickness (t) are shown. The results clearly reflect that the surface plasmon resonance is highly dependent on the geometrical ratio of the core/shell thickness. Thus allowing an additional degree of freedom for the optical tunability of such particles.

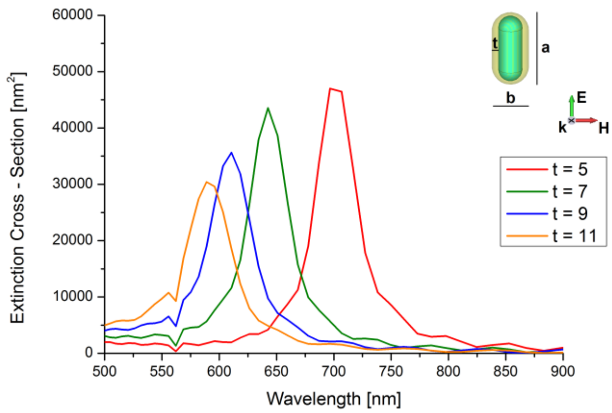

Fig. 2. Extinction spectra of the core/shell nanorod particle obtained by varying the shell thickness under longitudinal plasmon mode excitation. Geometrical parameters: $a = 80$; $b = 40$; $5 < t < 11$. All dimensions are expressed in nm.

We have also evaluated the near electric field distribution at the resonant wavelength as shown in Fig. 3.

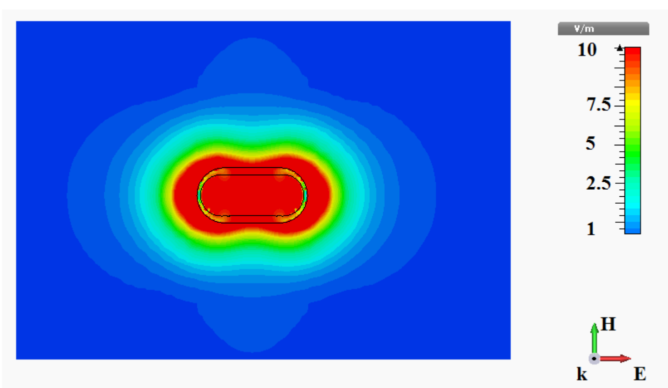

Fig. 3. Near electric field distribution of the core/shell nanorod particle at the resonant wavelength (696 nm) for: $a = 80nm$; $b = 40nm$; $t = 5nm$. The incident electric field amplitude is 1V/m.

This field distribution confirm us that the electromagnetic interaction between the proposed particle and the incident plane-wave results in a strong local electric field enhancement. In this way the local refractive index variation of the background environment produces a significant shift in the resonant wavelength of the particle.

III. Sensitivity Analysis

In this section we analyze the nanoparticle sensitivity properties by varying the thickness of the gold shell and the polarization of the incident plane wave.

The sensitivity is commonly defined as $S = \Delta\lambda/\Delta n$ expressed in nm/RIU (Refractive Index Unit). A test material, surrounding the nanoparticle, with a varying refractive index n in the range 1-1.6 has been chosen.

In table I and Table II the mean sensitivity values for the longitudinal and transverse plasmon mode excitation are respectively shown. The results reflect that the modified particle has a major sensitivity compared to the classical rod particle ($t \rightarrow b/2$) with the same volume.

TABLE I. Sensitivity performance of modified nanorod particle for different values of the shell thickness under longitudinal mode excitation.

Shell thickness	Resonant wavelength λ [nm]				Mean Sensitivity Values [nm/RIU]
	n=1	*n=1.2*	*n=1.4*	*n=1.6*	
t=5	696	785	867	969	455
t=7	642	706	785	867	375
t=9	610	668	738	810	333
t=11	588	642	706	772	306
$t \rightarrow b/2$	562	610	668	727	275

TABLE II. Sensitivity performance of modified nanorod particle for different values of the shell thickness under transverse mode excitation.

Shell thickness	Resonant wavelength λ [nm]				Mean Sensitivity Values [nm/RIU]
	n=1	*n=1.2*	*n=1.4*	*n=1.6*	
t = 5	634	668	706	749	185
t = 7	581	610	634	668	145
t = 9	556	575	595	626	116
t = 11	530	549	568	595	108
$t \rightarrow b/2$	490	512	526	543	88

IV. Conclusion

In this paper a computational investigation of modified gold nanorod particles operating in the VIS and NIR was proposed.

The electromagnetic behavior of such particles are evaluated through full-wave numerical analysis. In particular, the extinction cross section spectra, near electric field distribution and sensitivity performance for both longitudinal and transverse modes excitation was presented.

These results encourage a possible use of such particles in array configuration for biosensing application.

References

[1] A. Moores and F. Goettmann, "The plasmon band in noble metal nanoparticles: an introduction to theory and applications," *New J. Chem.*, vol.30, no.8, pp. 1121-1232, 2006.

[2] S. Li, S. Yin, Y. Jiang, C. Yin, Q. Deng and C. Du, "Specific Protein Detection in Multiprotein Coexisting Environment by Using LSPR Biosensor," *IEEE Trans. on Nanotechnology*, vol.9, no.5, pp. 554-557, 2010.

[3] W. Cai, T. Gao, H. Hong and J. Sun, "Applications of gold nanoparticles in cancer nanotechnology," *Nanotechnology, Science and Applications*, vol.1, pp. 17-32, 2008.

[4] K.C. Chu, C.Y. Chao, Y.F. Chen, Y.C. Wu and C.C. Chen, "Electrically controlled surface plasmon resonance frequency of gold nanorods," *App. Phy. Lett.*, vol.89, no.10, pp. 103107-103107-3, 2006.

[5] P.K. Jain, K.S. Lee, I.H. El-Sayed and M.A. El-Sayed, "Calculated Absorption and Scattering Properties of Gold Nanoparticles of Different Size, Shape, and Composition: Applications in Biological Imaging and Biomedicine," *J. Phys. Chem.*, vol.110, no. 14, pp. 7238-7248, 2006.

[6] P.B. Johnson and R.W. Christy, "Optical Constants of the Noble Metals," *Phys. Rev. B*, vol.6, no.12, pp. 4370-4379, 1972.