Numerical investigation of plasmonic properties of gold nanoshells

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ABSTRACT

We numerically investigated plasmonic properties of gold coated 300 nm core shell particles (CS). It is known that the surface plasmon decays into the medium that encompasses the metal nanoparticle. This decay converts changes in the local refractive index into a frequency shift of the SPR. In this work, the core material was polystyrene and the shell was a thin gold layer. We showed that this CS exhibits two plasmonic modes in the visible-near infrared regime. The blue end plasmonic mode was confined at the core-metal dielectric interface and the red end plasmonic mode was attributed to a surface mode that depends on dielectric properties of the surrounding medium. The application of the red end plasmonic mode as a surface plasmon resonance (SPR) sensor revealed that it exhibits wavelength shift of 764±13 nm per refractive index unit change of the surrounding medium (nm/RIU). Potential biomedical applications of these sensors are discussed.
Keywords: Surface plasmon, nanoshell, finite element, resistive heating

1. INTRODUCTION

Surface plasmon (SP) represents an oscillation of collection of free electrons at the metal-dielectric interface. The dispersion relation of the surface plasmon is given by $k_{sp} = \frac{\omega}{c}\left(\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}\right)^{1/2} = k_o\left(\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}\right)^{1/2}$, where ω is the angular frequency of the incident radiation, k_o is the free space wavevector, and ε_m and ε_d are the dielectric functions of the metal and the dielectric medium, respectively[1-2]. The excitation of SP depends on dielectric properties of the medium adjacent to metal. This property of SP has long been explored for real-time, label-free detection and this technology and has reached a stage of high throughput bio-sensing using array format in the SPR microscope[3]. SPR sensors also find applications in other fields that include biotherapeutics, drug discovery research, biomolecular interactions and food quality safety analysis[2].

Recently core shell particles have found applications in the biomedical field[4-6]. The advantage of using core-shell particles is that it exhibits plasmon excitation at the near-infrared regime where optical transmission through tissue is optimal[4-7]. Moreover, the nanoshell configuration is more sensitive to the surrounding environment compared to a solid metallicnanoparticle[7]. Understanding how the plasmon excitation is modified when changing the shell thickness or composition, or the core material of the CS, is important for the optimization of the particle design. We numerically investigated the plasmonic properties of CS using a finite element model. We studied the optical properties of core-shell of size about 300 nm containing polystyrene as the core and Au as shell in water. Finally we investigated potential applications of core shell as possible surface plasmon based wavelength resonance (SPR) sensors.

2. NUMERICAL METHODS

Numerical simulation was performed using Finite-Element Method. The finite element analysis package COMOSL (COMSOL, Burlington, MA, USA.) was used for all simulations. The simulations were performed by modeling the core-shell particle with a perfectly matched layer (PML) as outer boundary conditions. The surface boundary of the gold nanoshell was assigned far field condition. The dielectric properties of the material required for the numerical simulation were obtained from the Handbook of optical constants by Edward D. Palik[8].

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The refractive index of the PML is considered the same as refractive index of adjacent medium to prevent any reflection of the scattered waves from the boundary that enclosed the model. Meshing is other important parameter to be optimized carefully. Edges are meshed with maximum element size of 3 nm, boundaries are meshed symmetrically and the rest of geometry is meshed automatically using a finer mesh condition (figure 1(a)). The gold nanoshell was excited using a z polarised plane wave traveling in the x direction. The wave equation of the z polarised plane wave traveling in the x direction was given by $E_z = 1.\exp(-j*k_0*n*x)$, where k_0 is the free space wavevector and n is the refractive of the medium. The data of the far field variables were used to calculate total field using an embedded Straton-Chu formula. Figure 1(b) represents the resistive losses of the SP of a gold nanoshell that was excited by 830 nm light wave. Absorption cross section was obtained by integrating of the resistive heating over the nanoparticle volume.

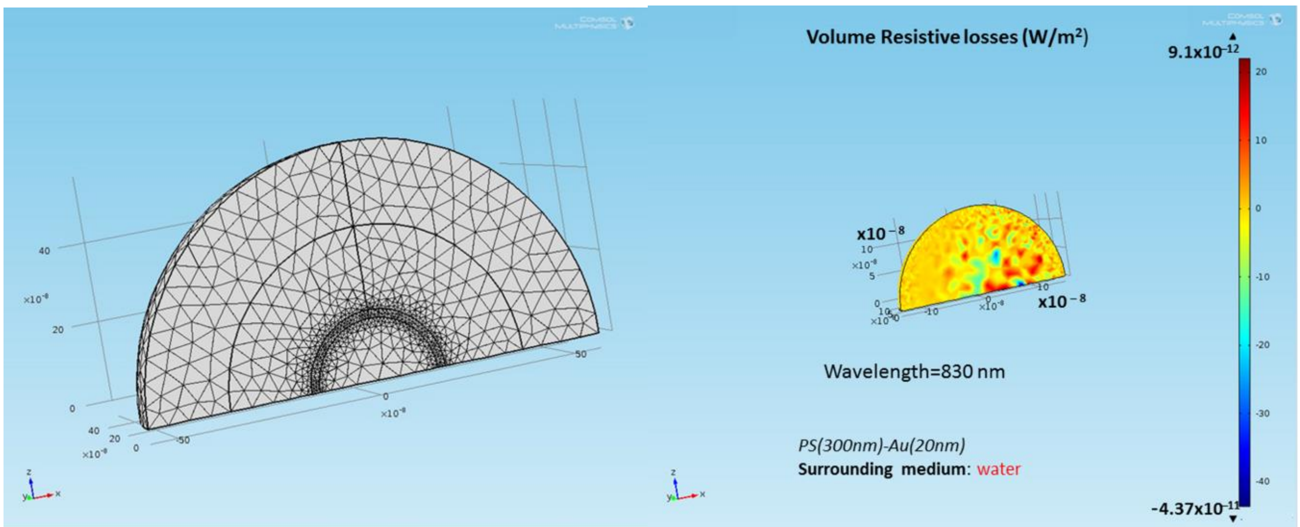

Figure 1. (a) Meshing of core shell nanoparticle and (b) Electric field distribution of SP around CS due to 830 nm light interaction.

Figure 1(b) represents the resistive losses of the SP of a gold nanoshell that was excited by 830 nm light wave. Absorption cross section was obtained by integrating of the resistive heating over the nanoparticle volume.

3. RESULTS

We studied the optical properties of a particle containing polystyrene as core and Au as shell in water. The core diameter was 300nm and the thickness of the shell was optimized for maximum SP excitation by increasing the shell thickness in steps of 10 nm from 20 nm to 50 nm. Figure 2 represents the optical absorption spectra of 300 nm polystyrene core particles with Au shell layer thicknesses 20 nm, 30 nm, 40 nm and 50 nm.

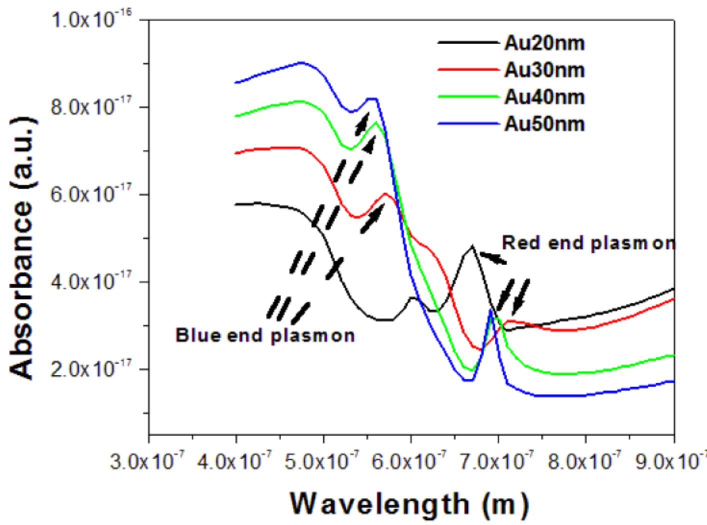

Figure 2. Numerically obtained optical absorption spectra of 300 nm core particles with Au shell thicknesses 20 nm, 30 nm, 40 nm and 50 nm.

A shell thickness in the range between 20 to 30 nm exhibits the maximum SP excitation. Two plasmonic modes, one at 600 nm corresponding to core–shell interface (inner mode) and the other at 670 nm corresponding to shell-surrounding dielectric interface (outer mode) were observed. Efficient plasmonic coupling between the two modes occurs when the size of the Au shell is between 20 to 30 nm.

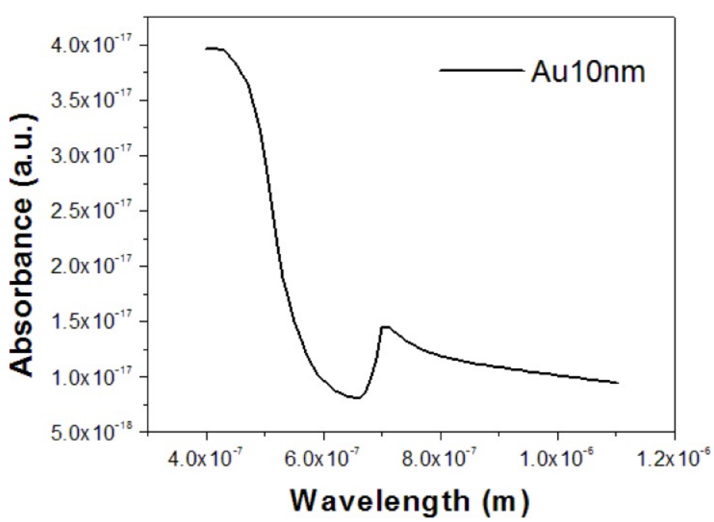

Figure 3. Numerically obtained optical absorption spectrum of CS of Au shell thickness 10 nm.

When the thickness of the Au shell is less than the skin depth (20 nm) of excited plasmon, only one prominent plasmonic mode is observed (figure 3).At a thickness greater than 30nm, two well separated plasmonic modes are observed. The outer plasmonic mode is broadened more than the inner mode as the shell thickness increased. This confirmed that the inner plasmonic mode is confined at the core-shell interface.

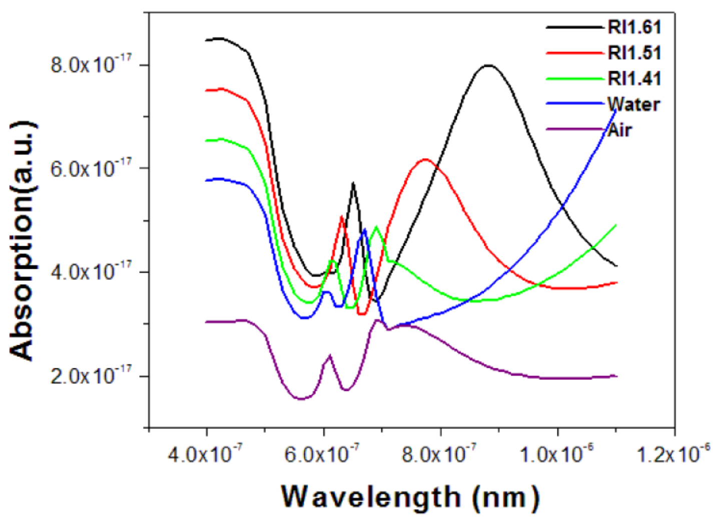

Figure 4. Optical absorption spectra of core shell in media of refractive indices (RI) air, water, 1.41, 1.51 and 1.61.

One of the CS applications for SPR sensors is investigated by simulating the CS particle in various refractive index media with refractive indices that varied from 1.33 (water) to 1.61.

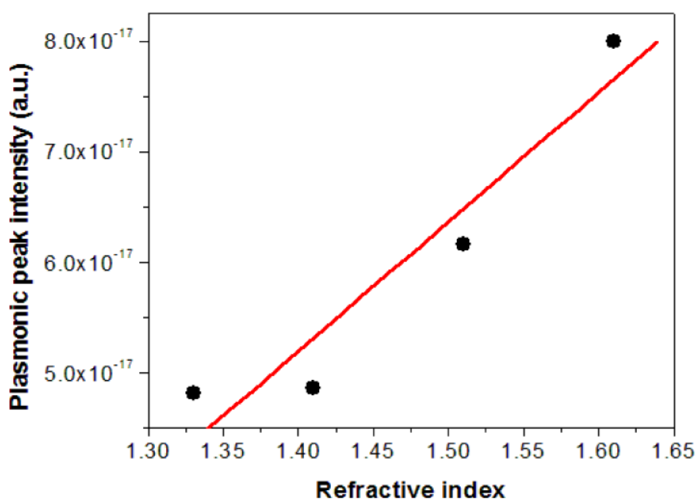

Figure 5. The change of the peak absorption wavelength of red end plasmonic mode (670 nm mode)as a function of the refractive index of the surrounding medium. The solid black dots represent the numerical simulated data and the solid red line represents a linear fit.

Figure 4 represents the optical absorption spectra of core shells in refractive index media that includes air, water, 1.41, 1.51 and 1.61. A red shift in wavelength and an increase in amplitude of absorption peak are observed.

The wavelength shift of the outer mode (670 nm) as function of refractive index was investigated. Figure 5 represents the wavelength shift of red end plasmonic mode or 670 nm mode due to change in the refractive index of the surrounding medium. The studies showed that the outer mode exhibits wavelength shift (dλ/dn) of 764±13 nm/RIU. The absorption of light by the red blood cell (RBC) is dominant by hemoglobin concentration and oxygen saturation level SnO_2, which determines the fraction of oxyhemoglobin and deoxyhemoglobin. Refractive index (RI) of RBC depends on its density and optical absorption property. Hemoglobin solution with concentration of 355.5 g/L exhibits RI between 1.413 to 1.438 for visible light[9]. Any change in blood concentration and oxygen level will induces refractive change in RBC which can be monitored using CS particles as SPR sensor as it exhibits wavelength shift of 764±13 nm/RIU.

4. CONCLUSION

We numerically investigated the plasmonic properties of 300 nm core shell particles. Two plasmonic modes were observed. Our investigation on the origin of plasmonic modes revealed that the electromagnetic field distribution of the blue end plasmonic mode was associated mainly with core-metal dielectric interface whereas the longer red end plasmonic mode was associated with surface of CS and was strongly influenced by its surrounding dielectric medium. The studies showed that the outer mode exhibits wavelength shift (dλ/dn) of 764±13 (nm/RIU) is comparable to most commonly used prism (970 (nm/RIU)) and grating (309 (nm/RIU)) based surface plasmon resonance techniques.

5. ACKNOWLEDGEMENTS

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