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Optimizing the figure of merit of gold nanoshell-based refractive index sensing

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ABSTRACT

In this article, the dependences of the refractive index sensitivity, linewidth, and figure of merit on the geometrical parameters of gold nanoshells are investigated by using the Mie theory of a coated sphere with the size-dependent dielectric function of metal nanoparticles. It is found that the hollow gold nanoshell have higher refractive index sensitivity as compared to the silica–gold nanoshell of the same dimensions. In addition, increasing core radius or decreasing shell thickness leads to a great improvement in the refractive index sensitivity, but it results in an excessive broadening of the linewidth, which make the detection of the resonance wavelength changes difficult. Therefore, the figure of merit is calculated to find optimal dimensions for gold nanoshells having the best sensing performance. The results show that the maximal figure of merit for the hollow gold nanoshell (2.59) is a little greater than that for the silica–gold nanoshell (2.50), and the optimal core radius and shell thickness, corresponding to the maximal figure of merit, of the hollow gold nanoshell (silica–gold nanoshell) are 31 and 7 nm (29 and 8 nm), respectively. The optimized gold nanoshells can be treated as potential candidates for chemical and biological sensing.

1. Introduction

Metal nanoparticles have found a wide range of applications because of their localized surface plasmon resonance (LSPR) and the ability to tune this resonance by changing the size, shape, composition, and surrounding medium of the nanoparticles [1]. LSPR is a coherent, collective spatial oscillation of the free electrons in a metal nanoparticle; it can be directly excited by light. When the LSPR is excited, metal nanoparticles strongly absorb and/or scatter the incident light upon them, and the local field around the nanoparticles is strongly enhanced. The light absorption properties of metal nanoparticles have been employed in the photothermal therapy, while the light scattering properties have been utilized for imaging [2]. In addition, the local field enhancement has been used in the surface enhanced Raman scattering [3] and surface enhanced fluorescence [4].

It is well known that the LSPR of metal nanoparticles is highly sensitive to the refractive index of the surrounding medium [5,6]. Therefore, nanoscale biological and chemical sensors have been developed using the shift of LSPR in response to changes in the local dielectric environment of the metal nanoparticles [7]. For the LSPR sensors, a strong shift in the LSPR wavelength in response to a relatively small change in the refractive index of the surrounding medium is required to ensure high sensitivity. In recent years, many excellent experimental and theoretical investigations [8–16] have been devoted to the LSPR sensitivity of metal nanoparticles with various shapes and sizes, in order to find the best nanoparticle configuration to improve the refractive index sensitivity (RIS), defined as the ratio of LSPR wavelength shift to the variation of the refractive index of the surrounding medium, for LSPR sensing applications. The results show that nanotriangles, nanorods, and nanoshells offer high RIS because the electrons in these nanostructures can be easily polarized by the light to the interface of the metal and medium [17]. Recent studies [18–20] have highlighted the importance of the linewidth (full width at half maximum, FWHM) of LSPR spectra in measurements of sensitivity, since a small FWHM is essential to improve the sensing resolution of LSPR sensing. Therefore, in addition to increasing RIS, the performance of a LSPR senor can be improved by narrowing FWHM. For this reason, a figure of merit (FOM) is defined as the ratio of RIS to FWHM in order to compare the overall performance of metal nanoparticles as sensors [21]. To improve the overall performance of metal nanoparticle-based sensors, it is necessary to optimize the geometrical parameters of nanoparticles to have maximal FOM for sensing applications. The optimization is an important first step in the ultimate selection of metal nanoparticles for sensing. To the best of our knowledge,

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no systematic investigation has ever been performed for the plasmonic sensing properties of gold nanoshells and no optimization has ever been carried out for the dimensions of gold nanoshells by maximizing the FOM. Therefore, the goal of this study is to fill this gap by providing quantitative analysis and optimization for the plasomonic sensing properties of gold nanoshells.

In this paper, the plasmonic sensing properties of gold nanoshells is studied by using the Mie theory of a coated sphere with the size-dependent dielectric function of metal nanoparticles. The effects of the core radius and shell thickness on the RIS, FWHM, and FOM are systematically simulated and quantitatively analyzed. To improve the performance of gold nanoshells for sensing applications, the maximal FOM and the corresponding optimal core radius and shell thickness are obtained.

2. Theory

2.1. Light extinction by the gold nanoshell

When a particle is illuminated by a beam of light, a part of the light is scattered by the particle, and another part of the light is absorbed if the particle is opaque. The total energy loss of the incident light is the sum of the scattered and absorbed energies by the particle. The scattered and absorbed energies are usually expressed by the scattering and absorption cross sections, C_{sca} and C_{abs}, respectively, and the total energy loss is expressed by the extinction cross section C_{ext} given by $C_{ext} = C_{sca} + C_{abs}$. The C_{ext} has the unit of area because it represent an equivalent cross sectional area of the particle that contributes to the scattering and absorption of the incident light.

The geometry of the gold nanoshell studied in this paper is shown in Fig. 1. The light extinction by the gold nanoshell is calculated by using the Mie theory of a coated sphere proposed by Aden and Kerker [22]. For the gold nanoshell, the extinction cross section is given by [23]

$$C_{ext} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\,Re\left\{a_n + b_n\right\}, \tag{1}$$

where k is the wavenumber in the surrounding medium, and a_n and b_n are the scattering coefficients. The a_n and b_n are the key parameters for the calculation of the extinction cross section; it can be calculated employing the algorithm proposed by Bohren and Huffman [23]. The required parameters for the calculation are the wavelength of incident light λ, the core radius R_1, the shell thickness t (or the shell radius R_2), and the refractive indices of the core, shell, and surrounding medium, n_1, n_2, and n_m, respectively. In our calculations, the core of the gold nanoshell was considered to be silica with refractive index given by Malitson [24] or vacuum with refractive index of 1.0. The refractive index of the gold shell (n_2) can be obtained from the dielectric function ε of the gold shell by $n_2 = \varepsilon^{1/2}$. The calculation of the dielectric function for the gold shell is described in the next subsection.

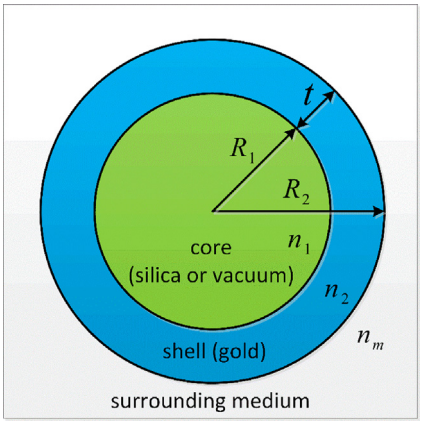

Fig. 1. Geometry of gold nanoshell. R_1, R_2, and t are the core radius, shell radius, and shell thickness, respectively. n_1, n_2, and n_m are the refractive indices of the core, shell, and surrounding medium, respectively.

2.2. Size-dependent dielectric function

For bulk metals, the dielectric function is dependent on the angle frequency of the incident light (ω), and it is the sum of the contributions from the bound and free electrons in the metals,

$$\varepsilon_{bulk}(\omega) = \varepsilon_{bound}(\omega) + \varepsilon_{free}(\omega), \tag{2}$$

where ε_{bound} and ε_{free} originate from the interband and intraband transitions, respectively. The contributions from the free electrons can be described by the Drude model [23],

$$\varepsilon_{free}(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma_{bulk}}, \tag{3}$$

where ω_p is the plasma frequency, and $\gamma_{bulk} = v_f/l_\infty$ is the bulk collision frequency dependent on the Fermi velocity v_f and the mean free path of the free electrons l_∞.

The dielectric function of a bulk metal is independent on size. However, when the light interacts with the small metal nanoparticles of the size smaller than the mean free path of the free electrons, the dielectric function of the nanoparticles deviates from the bulk value. The bulk collision frequency increases because the collision of the free electrons with the particle surface becomes important as an additional relaxation process and cannot be neglected [25]. Therefore, when the size-dependent free electron surface scattering become important, the bulk collision frequency should be modified as follows,

$$\gamma = \gamma_{bulk} + Av_f/L_{eff}, \tag{4}$$

where A is a dimensionless parameter which is usually assumed to be close to 1, and L_{eff} is the effective mean free path of the free electrons dependent on the dimensions of the metal nanoparticles. Thus, for small metal nanoparticles, the dielectric function should be modified to account for the surface scattering of the free electrons, which is expressed as

$$\begin{aligned}\varepsilon(\omega, L_{eff}) &= \varepsilon_{bound}(\omega) + \varepsilon_{free}^{nano}(\omega, L_{eff})\\ &= [\varepsilon_{bulk}(\omega) - \varepsilon_{free}(\omega)] + \varepsilon_{free}^{nano}(\omega, L_{eff})\\ &= \varepsilon_{bulk}(\omega) + \frac{\omega_p^2}{\omega^2 + i\omega v_f/l_\infty} - \frac{\omega_p^2}{\omega^2 + i\omega(v_f/l_\infty + Av_f/L_{eff})}.\end{aligned} \tag{5}$$

For gold nanoshells, $\hbar\omega_p = 9.03$ eV [26], $v_f = 1.40 \times 10^{15}$ nm/s [27], $l_\infty = 42$ nm [27], $A = 1$ [27], $L_{eff} = t$ [27], and the values of the bulk dielectric function ε_{bulk} were obtained from the literature reported by Johnson and Christy [28].

3. Results and discussion

The response of the extinction spectrum and LSPR wavelength of a gold nanoshell with core radius of 30 nm and shell thickness of 10 nm to the refractive index of the surrounding medium is shown in Fig. 2. It is seen that the extinction spectrum redshifts as the refractive index of the surrounding medium is increased from 1.0 to 1.6, along with an increase in the intensity of the extinction resonance peak (Fig. 2(a) and (c)). The LSPR wavelength (i.e., the position of the extinction resonance peak) increases linearly with increasing the medium refractive index, and the silica–gold