Optics Communications 349 (2015) 193–197

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Gold nanoshells with gain-assisted silica core for ultra-sensitive bio-molecular sensors

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ARTICLE INFO

Article history:
Received 30 January 2015
Received in revised form
3 March 2015
Accepted 25 March 2015
Available online 27 March 2015

Keywords:
Spherical core–shell nanoparticle
Gain
Optical cross section
Bio-molecular sensors

ABSTRACT

A novel bio-molecular nanostructured sensor composed of Au spherical nanoshell and gain-assisted silica-core has been proposed and investigated theoretically, which shows a superior performance compared to the existing structured sensor. Using quasi-static approximation calculation, it is found that the scattering efficiency and the quality factor of SPR can be enhanced greatly by introducing proper amount of gain. The simulated results demonstrate that our designed Au spherical nanoshell and gain-assisted silica-core can obtain as high as 166.7 nm/RIU for the sensitivity of refractive index, and the sensors' figure of merit is enhanced 2000 times nearly compared to that of $g=0$, which indicates that the designed spherical core–shell sensors have the powerful ability to detect a subtle change in the concentration of its background medium.

1. Introduction

In the last two decades, great interests have been focused on the development of spherical shell nanoparticles that composed of a dielectric core and a coating metal shell. Spherical shell nanoparticles can be designed to meet specific applications because of its optical signature and physical properties [1,2]. A very important optical phenomenon, the surface plasmon resonance (SPR), which is excited at metal surface by electromagnetic waves coupling with charge oscillations [3,4], has attracted lots of researching attentions. Incident photons can be localized in the surface of the metal nanoparticles, which will lead to enormous enhancement of the optical local field in nanoscale. This great enhancement makes particles be sensitive to the refractive index of the surrounding medium extremely, which forms the basis for SPR sensing [5,6]. Another, a relatively simple geometry of the spherical shell structure can obtain a wider plasmonic tunability compared to the simplex metal nanoparticles [3,7–9]. For these reasons, different spherical shell nanoparticles or nanostructures have been applied extensively in bio-molecular sensors [5], photothermal therapy [10], and bio-imaging [11].

A relatively low quality factor of SPR, which derives from high dissipative losses on metallic component of spherical shell nanoparticles, is a main reason to restrict the applications of SPR in sensing or switching [12]. By introducing the gain into the coating of silica (shell) coated gold (core) nanosphere, the energy of the gain medium can be transferred to the metallic component to completely compensate the ohmic losses and thus the scattering efficiency can be typically increased [9,13]. However, the existing silica shell layer will hinder direct contact between the metal particle and the surrounding medium, resulting in the enhancement of the local field cannot completely exposed to the surrounding medium, which will reduce the sensitivity of SPR bio-molecular sensors [14]. Meanwhile, the gain in silica shell layer could be destroyed by the interactions with various background media [15]. One promising scheme can be a gold (shell) coated gain-assisted silica (core) nanosphere structure, where the gold shell layer can contact the surrounding medium fully, and the gold shell layer protect the core material from being affected by different surrounding medium.

In this paper, we incorporated a suitable amount of gain in core layer to improve the sensitivity of the gold-shell silica–core nanoparticle for bio-molecular sensors. Using quasi-static approximation calculation, the simulated results show that a proper level of gain incorporated in the core layer strongly enhances the scattering efficiency as well as the quality factor of SPR. Indeed, the structure of both the coating metal layer and a gain-assisted silica-core can obtain a great improvement of performance in bio-molecular sensors, which has been investigated and demonstrated by quantitative analysis. The simulated results show that a high refractive index (RI) sensitivity of 166.7 nm/RIU and a 2000 times' increase in figure of merit of sensors compared to that of $g=0$ can be obtained in our designed scheme. Our results confirm that the

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http://dx.doi.org/10.1016/j.optcom.2015.03.061
0030-4018/

designed spherical core–shell sensors have the powerful ability to detect a subtle change in the concentration of its background medium.

2. Design and analysis method

The designed structure is shown in the inset of Fig. 1, which is composed of an Au spherical nanoshell and a gain-assisted silica-core. The effective refractive index of gain-introduced silica core can be expressed as $n_c = 1.43 - ig$, where the imaginary part (g) represents the level of optical gain coefficient. In experiments, the coefficient of gain medium can be modulated by the methods of optically pumped [16] or electrically injected [17]. The effective permittivity of gold-shell can be obtained by the Drude-model and can be expressed as $\varepsilon_s = \varepsilon_\infty - \omega_p/(\omega^2 + i\omega\Gamma)$, where $\omega = 2\pi f$ is the angular frequency, $\omega_p = 1.37 \times 10^{16}$ rad/s is the plasma frequency, $\varepsilon_\infty = 9.5$, and Γ is the collision frequency [18]. Since the depth of the Au nanoshell is thinner than the electron mean free path in bulk Au, the electron surface scattering cannot be ignored. When size-dependent electron scattering becomes important, the effective collision frequency can be modified as follows [7]:

$$\Gamma = \gamma_{bulk} + Av_F/R \tag{1}$$

where $\gamma_{bulk} = 3.33 \times 10^{13}\,\mathrm{s}^{-1}$ is the bulk collision frequency, $v_F = 1.40 \times 10^8$ cm/s is the Fermi velocity, A is a parameter determined by the geometry and theory used to derive this expression [19] (for simple Drude theory and isotropic scattering, A=1), and $R = r_2 - r_1$ is the reduced electron mean free path. The r_1 and $r_2 - r_1$ are the radius of the dielectric core and the depth of the Au shell, respectively.

We assumed that the gold-shell silica–core nanoparticle is suspended in a homogeneous isotropic background medium, and its size is smaller than the wavelength of the incident light. Then, the phase retardation of the incident light, caused by interacting with the nanoparticle, can be ignored. So quasi-static approximation theory can be employed for characterizing the nanoparticles' electromagnetic performance. According to the quasi-static approximation theory, the induced dipole inside the nanoparticle by the incident electric field can be expressed as $P = \alpha E_0$ The polarizability α can be given as follows [3]:

$$\alpha = 4\pi r_2^3 \frac{r_1^3(\varepsilon_c - \varepsilon_s)(2\varepsilon_s + \varepsilon_b) + r_2^3(\varepsilon_c + 2\varepsilon_s)(\varepsilon_s - \varepsilon_b)}{2r_1^3(\varepsilon_c - \varepsilon_s)(\varepsilon_s - \varepsilon_b) + r_2^3(\varepsilon_c + 2\varepsilon_s)(\varepsilon_s + 2\varepsilon_b)} \tag{2}$$

where $\varepsilon_c = n_c^2$ and $\varepsilon_b = n_b^2$ are the relative permittivities of the

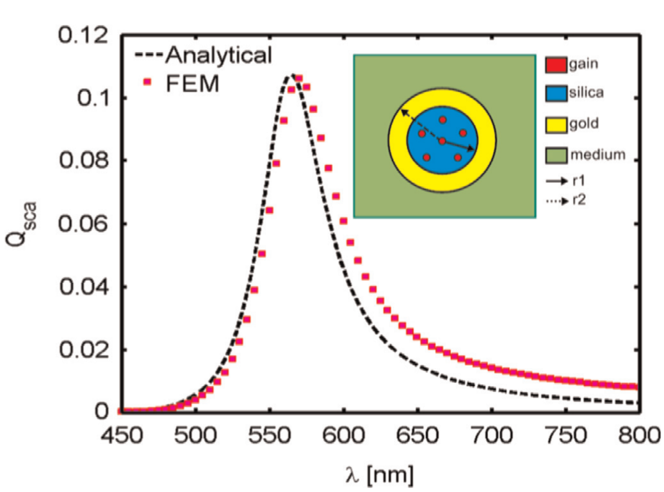

Fig. 1. Scattering efficiency of spherical shell nanoparticle without gain ($n_b = 1$). Inset shows the schematic of spherical shell nanoparticle.

dielectric core and the background medium, respectively. Finally, we can obtain the scattering coefficient from the polarizability by using a scattering theory, where the scattering coefficient is defined as the ratio of the scattering cross-section to the projective cross-section of the particle. Therefore, the scattering coefficient can be expressed as follows:

$$Q_{sca} = \frac{\sigma_{sca}}{\pi r_2^2} = \frac{k_b^4}{6\pi^2 r_2^2}|\alpha|^2 \tag{3}$$

where $k_b = 2\pi n_b/\lambda$ is the wave number in the background medium, λ is the wavelength of the incident light in the free space.

The core radius, the nanoshell thickness and the total radius of the designed spherical shell nanoparticles are set as $r_1 = 15$ nm, $r_2 - r_1 = 5$ nm and $r_{total} = r_2 = 20$ nm, respectively, which is less than 1/20 of the wavelength in free space, so the quasi-static approximation calculation is applicable. Therefore, the scattering coefficient for the designed spherical shell nanoparticle without the gain (g=0), can be obtained according to Eqs. (2) and (3) as shown in Fig. 1. Here, for simplicity, the background medium is set as the vacuum with $n_b = 1$. In Fig. 1, we can observe that a clear scattering peak appears at the wavelength of 564.5 nm with peak scattering coefficient of about 0.1073.

The accuracy of the above results by quasi-static approximation can be verified based on the finite elements method. The relative scattering cross-section can be obtained from the scattered field, which is defined via Poynting's theorem [20]:

$$\sigma_{sca} = \frac{P_{sca}}{I_{inc}} = \frac{1}{I_{inc}}\mathrm{Re}\left\{\frac{1}{2}\oiint_S\left[\overrightarrow{E_S} \times \overrightarrow{H_S}\right]\cdot\hat{n}dS\right\} \tag{4}$$

where S is the sphere that surrounds the nanoparticle, $\hat{n}$ is the normal vector pointing to the surface, I_{inc} is the incident intensity, $\overrightarrow{E_S}$ and $\overrightarrow{H_S}$ are the scattered electric and magnetic fields. Finally, the scattering coefficient can be calculated by Eq. (3) as shown in Fig. 1 in the dotted line. Obviously, the numerical simulations result agrees well with the one calculated by quasi-static approximation, which means quasi-static approximation have a high accuracy on calculating the proposed nanoparticles.

Fig. 2(a) shows the scattering coefficient of the proposed nanostructure as a function of optical gain (g) and wavelength (λ) using quasi-static approximation analysis. Considering the actual application environment of SPR sensors, the background medium is set as the water ($n_b = 1.333$) instead of the vacuum. It is seen that the peak of the scattering coefficient increase smoothly at $0 \le g \le 0.4$. When g arrives to a suitable point, the value of the scattering coefficient can reach to its maximum (the peak) drastically, and then it falls down as g increases. This trend can be also seen more clearly in Fig. 2(b), where g takes some special numbers. When $g = 0.471$, an extremely narrow peak appears, and the scattering coefficient reaches to the maximum as high as 1.18×10^6, which is over 10^6 times higher than that of the same structure without any gain ($g = 0$). The results indicate that the losses associated with the nanoparticle can be compensated, and even can be surpassed by the gain, so that the extinction cross section is dominated entirely by scattered radiation. From Fig. 2 (a) and (b), we can also find that, no matter how g changes, the wavelength of the peak position of the scattering coefficient do not shift nearly because of the intrinsic plasmonic resonance of the nanoparticle.

For a further illustration, the relationship between the peak heights of the scattering coefficient and the gain (g) is shown in Fig. 2(c), where it is seen that a suitable number of gain is the key to achieve a high peak of the scattering coefficient. We also obtain the quality factor (QF) as a function of the g as show in Fig. 2(d), which is defined as ratio of the resonance wavelength to the full width at half maximum (FWHM) of resonance peak,