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Optimal dimensions of gold nanoshells for light backscattering and absorption based applications

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ABSTRACT

Gold nanoshells, a novel type of composite spherical nanoparticle consisting of a spherical dielectric core covered by an ultrathin gold shell, have been used as contrast agents for biological imaging as well as therapeutic agents for photothermal therapy based on their strong backscattering and absorption properties. In this paper, we investigate the dependence of the backscattering and absorption properties of silica core–gold nanoshells on the core radius and shell thickness by using the Mie theory for a coated sphere with the size-dependent dielectric function of metal nanoparticles. Our results show that, by varying the core radius and shell thickness, the position and intensity of the backscattering and absorption resonance peak can be tuned within the visible and near-infrared regions. We obtain the optimal dimensions of silica core–gold nanoshells for light backscattering and absorption based applications: biological imaging, photothermal therapy, and combined biological imaging and photothermal therapy. The optimized gold nanoshells can be used as ideal contrast and therapeutic agents.

1. Introduction

Metal nanoparticles are able to strongly absorb and scatter light within the visible and near-infrared wavelength regions. It is attributable to the localized surface plasmon resonance (LSPR) of metal nanoparticles while interacting with light. When the LSPR of metal nanoparticles is excited, absorption and scattering of light by nanoparticles as well as the local electric field around the nanoparticles are strongly enhanced. The resonance wavelength and the extent of enhancement are dependent on the size, shape, and dielectric environment [1]. In addition, they are also dependent on the spacing between the nanoparticles and the polarization of the incident light [2]. These special optical properties of metal nanoparticles make them have tremendous potential applications in many research fields, including biological imaging [3], photothermal therapy [4], biosensing [5], surface enhanced Raman scattering (SERS) [6], and photovoltaic devices [7].

Gold nanoshells, consisting of a nanoscale dielectric core coated with an ultrathin gold shell, are a novel type of composite metal nanoparticles invented by Halas et al. [8,9]. By varying the dimension and composition of each layer of the nanoshell structure, the resonance wavelength can be tuned to any wavelength desired across a large region of the visible and near-infrared spectra, and the extent of light absorption and scattering enhancement can also be tuned [8–11]. Owing to these advantages, gold nanoshells have been used as therapeutic agents for photothermal cancer therapy based on their strong absorption in the near-infrared region [12–16]. Hirsch et al. [12] were the first to demonstrate the photothermal cancer therapy using gold nanoshells. Gold nanoshells have been tested as targeted-therapy probes for human breast [13], prostate [14], brain [15], and liver [16] cancers. In addition to their potential applications as therapeutic

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agents, gold nanoshells have also been used as contrast agents for biological imaging with optical coherence tomography (OCT) due to their strong backscattering in the near-infrared region [17–21]. Loo et al. [17] were the first to demonstrate the feasibility of using gold nanoshells as contrast agents for biological imaging with OCT. Agrawal et al. [18] investigated the influence of geometry and concentration of gold nanoshells on OCT signal enhancement in turbid media by *in vitro* OCT measurements. Their experimental results indicated that gold nanoshells with high backscattering are the effective contrast agents for OCT imaging. Zagaynova et al. [19] demonstrated the efficiency of gold nanoshells as contrast agents for OCT imaging of agar biotissue phantoms and rabbit skin *in vivo*. Kah et al. [20,21] studied the dependence of concentration of gold nanoshells on OCT signal enhancement. They found that too high a concentration of gold nanoshells only enhances the OCT signal near the tissue surface, while significantly attenuating the signal deeper into the tissue. Recently, Gobin et al. [22] have demonstrated the feasibility of using gold nanoshells for combined biological imaging and photothermal therapy. Strong backscattering is essential for biological imaging, while effective photothermal therapy requires high absorption. Thus the optimal design of gold nanoshells in the near-infrared region is an important first step in the ultimate selection of gold nanoshells for biological imaging and photothermal therapy. Therefore, the main goal of this study is to obtain the optimal dimensions of gold nanoshells for the above-mentioned backscattering and absorption based applications: biological imaging, photothermal therapy, and combined biological imaging and photothermal therapy.

In this paper we investigate the effects of the core radius and shell thickness on the backscattering and absorption properties of gold nanoshells by using the Mie theory of a coated sphere with the size-dependent dielectric function of metal nanoparticles, and we obtain the optimal dimensions of gold nanoshells. This paper is organized as follows. Section 2 introduces the calculation of the backscattering and absorption cross sections of gold nanoshells by using Mie theory of a coated sphere with the size-dependent dielectric function of metal nanoparticles. In Section 3, the effects of the core radius and shell thickness on the absorption and backscattering spectra are investigated, and optimal core radii and shell thicknesses of gold nanoshells are obtained. Section 4 is devoted to the conclusion.

2. Theory

2.1. Backscattering and absorption of gold nanoshells

In this work we have considered and studied the gold nanoshells with geometries shown in Fig. 1. The backscattering and absorption properties of an individual gold nanoshell can be described by the backscattering and absorption cross sections, C_{back} and C_{abs}. The C_{back} is defined as the ratio of scattered power in a unit solid angle around the backscattering direction to intensity of incident light, and the C_{sca} is defined as the ratio of total scattered power to intensity of incident light. The C_{back} is a part of the C_{sca}. The C_{abs} is defined as the ratio of the absorbed power by the particle to the intensity of incident light. The C_{back} and C_{abs} represent equivalent cross sectional areas of the particle that contributes to backscattering and absorption of the incident light, respectively. The C_{back} and C_{abs} of an individual gold nanoshell can be calculated by using Mie theory of a coated sphere [23]

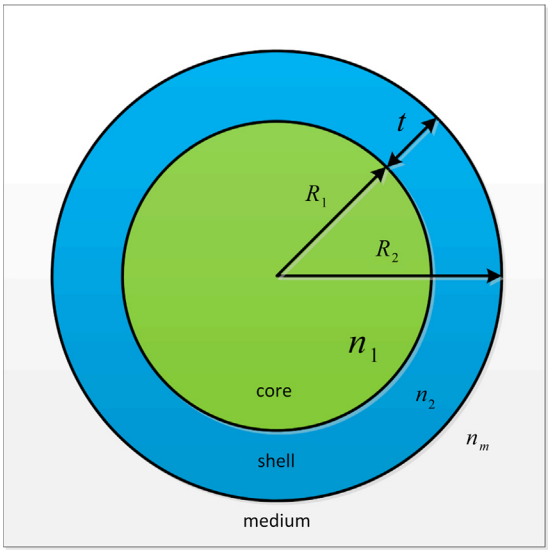

Fig. 1. Schematic of a gold nanoshell. R_1, R_2, and t are the core radius, shell radius, and shell thickness, respectively. n_1, n_2, and n_m are the refractive indices of the core, shell, and surrounding medium, respectively.

$$C_{back} = \frac{1}{4k^2}\left|\sum_{n=1}^{\infty}(2n+1)(-1)^n(a_n - b_n)\right|^2, \tag{1}$$

$$C_{abs} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\left[\mathrm{Re}(a_n + b_n) - |a_n|^2 - |b_n|^2\right], \tag{2}$$

where k is the wavenumber in the surrounding medium, and a_n and b_n are the scattering coefficients which can be calculated by employing the algorithm proposed by Bohren and Huffman [24].

The backscattering and absorption properties of an ensemble of gold nanoshells can be described by the backscattering and absorption coefficients, μ_{back} and μ_{abs}, which represent the total backscattering and absorption cross sections of gold nanoshells within unit volume, respectively. If multiple scattering is negligible and the gold nanoshell ensemble is monodisperse (i.e., the gold nanoshells have the same dimensions), the μ_{back} and μ_{abs} are given by

$$\mu_{back} = NC_{back} = f\frac{C_{back}}{V_p}, \tag{3}$$

$$\mu_{abs} = NC_{abs} = f\frac{C_{abs}}{V_p}, \tag{4}$$

where N is the particle number density (i.e., the number of particles per unit volume), f is the volume fraction of particles (i.e., the volume of particles per unit volume), V_p is the volume of an individual particle. In this paper, we