Optics Communications 284 (2011) 1076–1081

Contents lists available at ScienceDirect

Optics Communications

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

Scattering properties of an individual metallic nano-spheroid by the incident polarized light wave

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ARTICLE INFO

Article history:
Received 6 August 2010
Received in revised form 16 September 2010
Accepted 13 October 2010

Keywords:
Metallic nano-spheroid
Scattering properties
3D boundary element method

ABSTRACT

The scattering properties of a metallic nano-spheroid under the illumination of different polarized light waves are investigated using 3D boundary element method. The influences of different geometrical sizes of the nano-spheroid and incident directions of the illuminating light wave on the scattering spectrum are studied for different incident polarized light waves. The results show that the metallic nano-spheroid has two intrinsic resonant modes, corresponding to different polarization states and resonant wavelengths. The scattering enhancement, the resonant wavelength, and the location of the enhanced optical field are strongly dependent on the polarization properties of the illuminating light waves, and they can be modulated by appropriately choosing the polarization directions of the incident light wave.

1. Introduction

The local field enhancements and scattering properties of metallic nanoparticles at certain wavelengths or wavelength range can be used in many regions, such as photothermal destruction of cancer cells [1], optical antenna [2], chemical and biological sensors [3], cloaking [4], surface-enhanced Roman spectroscopy (SERS) [5–7], aperture-less near-field optical microscopy [8] and so on. The geometrical shapes and sizes of the metallic nanoparticles interested include the highly symmetrical structures, for instance sphere, and the partial symmetrical ones, such as spheroid, and the optical scattering properties of the highly symmetrical nano-sphere are not sensitive to the polarization of the incident light wave. The optical scattering behaviors of the lower symmetrical nano-spheroid can be influenced by the polarization of the incident light wave. For a metallic elongated nano-spheroid, it is reported that at resonant wavelength the localized electric field intensity very close to the sharp tips of the nano-spheroid can be hundreds of times of that of the incident light wave [9].

The optical properties of metallic nano-spheroids have been investigated [9–17] using Mie–Gans theory [18,19] or using numerical methods such as discrete dipole approximation (DDA). The results show that the size of the nano-spheroid, the proportion between the major axis and the minor axis, as well as the incident direction of the illuminating linearly polarized light can influence its scattering spectrum [9–11]. However, major attention is paid on the longitudinal and the transversal SPP modes, and other polarization directions are few discussed [9–11], and the circularly and elliptically polarized light are few investigated, either. In actual applications, when the nanoparticle is fabricated and its geometrical size is fixed, it is important to know whether the scattering behaviors and the optical field distributions can be modulated by the available approaches such as the polarization direction of the illuminating polarized light wave, and how the incident angle of the illuminating light and the geometrical shape and size of the nano-spheroid affect its optical scattering behaviors when the polarization of the incident light wave is fixed.

In this paper, the scattering spectra of a single metallic nano-spheroid for different polarization directions of the incident polarized light wave are investigated by 3D boundary element method (BEM) [20–22]. Two intrinsic SPP modes corresponding to the resonant wavelengths of the metallic nano-spheroid are studied. It is also exploited that the modulation of the scattering spectrum of the metallic nano-spheroid is feasible by the incident polarized light wave, and the incident angle of the illuminating light wave can be employed to adjust the scattering spectrum in certain polarization directions as well.

This paper is organized as follows: in Section 2, the 3D BEM is briefly revisited, and the scattering cross section (*SCS*) is defined. In Section 3, the scattering properties of the metallic nano-spheroid under the illumination of different polarized light waves with different polarization directions and incident directions are studied in detail. Brief conclusions are drawn in Section 4.

2. Basic formulas of 3D BEM

The 3D scattering problem can be schematically shown in Fig. 1. Suppose that the surface Γ of a particle divides the whole space into two parts: the inner part V_1 and the outer part V_2, and both parts are filled with homogenous medium of dielectric constant ε_i and permeability μ_i, where the subscript $i=1$ or 2 represents the variant

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doi:10.1016/j.optcom.2010.10.033

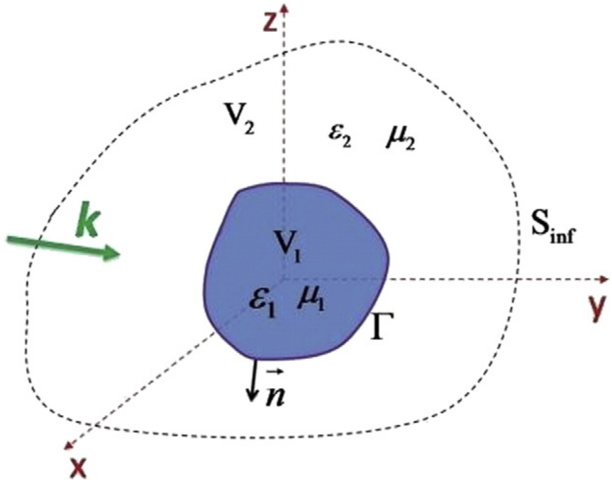

Fig. 1. Sketch of a single particle scattered by the incident light wave. The regions inside and outside the particle are noted as V_1 and V_2, respectively. The dielectric constants and the permeability are ε_1,μ_1 in V_1, and ε_2,μ_2 in V_2, respectively. Γ represents the surface of the particle, and $S_{\inf}$ denotes the surface of V_2 at infinity. $\vec{n}$ denotes the unit normal vector of the boundary surface Γ.

in region V_1 or region V_2. The incident light $\vec{H}_{inc}$ is scattered by the particle.

From rigorous Maxwell's equations, one can obtain the following vector integral equations for determining the magnetic field distribution $\vec{H}_i(\vec{r_i})$ in region V_i ($i=1, 2$) as

$$\begin{cases} -\oint_\Gamma j\omega\varepsilon_1 G_1(\vec{r_1}, \vec{r_\Gamma})\, \vec{n}\times \vec{E_1}(\vec{r_\Gamma}) + \vec{n}\times \vec{H_1}(\vec{r_\Gamma}) \\ \quad \times \nabla G_1(\vec{r_1}, \vec{r_\Gamma}) + \vec{n}\cdot \vec{H_1}(\vec{r_\Gamma})\nabla G_1(\vec{r_1}, \vec{r_\Gamma}) dS_\Gamma = \vec{H_1}(\vec{r_1}), & (1) \\ \vec{H}_{inc}(\vec{r_2}) + \oint_\Gamma j\omega\varepsilon_2 G_2(\vec{r_2}, \vec{r_\Gamma})\, \vec{n}\times \vec{E_2}(\vec{r_\Gamma}) + \vec{n}\times \vec{H_2}(\vec{r_\Gamma}) \\ \quad \times \nabla G_2(\vec{r_2}, \vec{r_\Gamma}) + \vec{n}\cdot \vec{H_2}(\vec{r_\Gamma})\nabla G_2(\vec{r_2}, \vec{r_\Gamma}) dS_\Gamma = \vec{H_2}(\vec{r_2}), & (2) \end{cases}$$

where $\omega = 2\pi f$ and $f = c/\lambda_0$ are the angle frequency and the space frequency of the light wave in vacuum, respectively. λ_0 and c are the wavelength and the velocity of the light wave in free space, respectively. $\vec{E_i}(\vec{r_\Gamma})$ and $\vec{H_i}(\vec{r_\Gamma})$ represent the electric field and the magnetic field on the surface boundary, respectively. The vectors $\vec{r_1}$, $\vec{r_2}$, and $\vec{r_\Gamma}$ correspond to the position vectors in region V_1, V_2, and at surface boundary Γ, respectively. $G_i = e^{-jk_i|\vec{r_i}-\vec{r_\Gamma}|} / (4\pi|\vec{r_i}-\vec{r_\Gamma}|)$ is the Green function, $k_i = 2\pi n_i/\lambda_0$ is the wave number and n_i is the refractive index of material in region V_i ($i=1, 2$).

Considering the boundary conditions

$$\begin{cases} \vec{E_t}(\vec{r_\Gamma}) = \vec{n}\times \vec{E_1}(\vec{r_\Gamma}) = \vec{n}\times \vec{E_2}(\vec{r_\Gamma}), & (3) \\ \vec{H_1}(\vec{r_\Gamma}) = \vec{H_2}(\vec{r_\Gamma}) = \vec{H}(\vec{r_\Gamma}) & (4) \end{cases}$$

and after removing the singularity [22], one can obtain the electromagnetic field distribution on the surface boundary as:

$$\begin{cases} -\oint_\Gamma j\omega\varepsilon_1 G_1(\vec{r_\Gamma}, \vec{r_\Gamma}')\vec{E_t}(\vec{r_\Gamma}') + \vec{n}\times \vec{H}(\vec{r_\Gamma}') \times \nabla G_1(\vec{r_\Gamma}, \vec{r_\Gamma}') \\ \quad + \vec{n}\cdot \vec{H}(\vec{r_\Gamma}')\nabla G_1(\vec{r_\Gamma}, \vec{r_\Gamma}') dS' = \frac{1}{2}\vec{H}(\vec{r_\Gamma}), & (5) \\ \vec{H}_{inc}(\vec{r_\Gamma}) + \oint_\Gamma j\omega\varepsilon_2 G_2(\vec{r_\Gamma}, \vec{r_\Gamma}')\vec{E_t}(\vec{r_\Gamma}') + \vec{n}\times \vec{H}(\vec{r_\Gamma}') \times \nabla G_2(\vec{r_\Gamma}, \vec{r_\Gamma}') \\ \quad + \vec{n}\cdot \vec{H}(\vec{r_\Gamma}')\nabla G_2(\vec{r_\Gamma}, \vec{r_\Gamma}') dS' = \frac{1}{2}\vec{H}(\vec{r_\Gamma}), & (6) \end{cases}$$

where $\vec{r_\Gamma}$ and $\vec{r_\Gamma}'$ denote the positions of the observation point and the source point at the surface boundary, respectively. The integral symbol $\oint_\Gamma dS'$ represents the Cauchy integral excluding singularity ($\vec{r_\Gamma} = \vec{r_\Gamma}'$).

Suppose that Γ is divided into M grids, after scalar processing of Eqs. (5) and (6) in Cartesian coordination, one can obtain $6M$ linear equations expressed as

$$A_{6M\times 6M}X_{6M\times 1} = B_{6M\times 1}, \tag{7}$$

$X_{6M\times 1}$ denotes the unknown components on x, y, and z directions of $\vec{E_t}$ and $\vec{H}$ to be solved on all the grids. $A_{6M\times 6M}$ is its coefficient matrix. $B_{6M\times 1}$ denotes the incident magnetic field on all the grids corresponding to each linear equation. The magnetic field and the tangential components of the electric field on boundary Γ can be determined by solving Eq. (7), and finally the total magnetic field over the whole space can be evaluated by Eqs. (1) and (2).

Suppose that there is a closed surface A (for instance, spherical surface) that surrounds the particle, and the outer normal vector of A is $\vec{n_A}$. SCS is defined as [23]

$$SCS = W_S / I_i, \tag{8}$$

where I_i is the incident light intensity. W_S denotes the electromagnetic energy crossing the surface A, written as

$$W_S = \int_A \vec{P}_{sca} \cdot \vec{n_A} dA', \tag{9}$$

where $\vec{P}_{sca}$ is the average Poynting Vector of the scattering field, described as

$$\vec{P}_{sca} = \frac{1}{2}\mathrm{Re}\left\{\vec{E}_{sca} \times \vec{H}^*_{sca}\right\}, \tag{10}$$

where $\vec{E}_{sca}$ and $\vec{H}_{sca}$ represent the scattering electric field and the scattering magnetic field, respectively.

3. Simulation results

A metallic nano-spheroid particle is sensitive to the polarization states of the incident light wave, so it is a good example to study how the scattering properties are influenced by various polarized light waves. The material of the metallic nano-spheroid in this paper is silver with the refractive index from Ref. [24]. The sketch of the nano-spheroid irradiated by the linearly polarized light wave is shown in Fig. 2. The lengths of the major axis and the minor axis of the nano-spheroid are equal to b and a, respectively, which are set as $b = 60$ nm

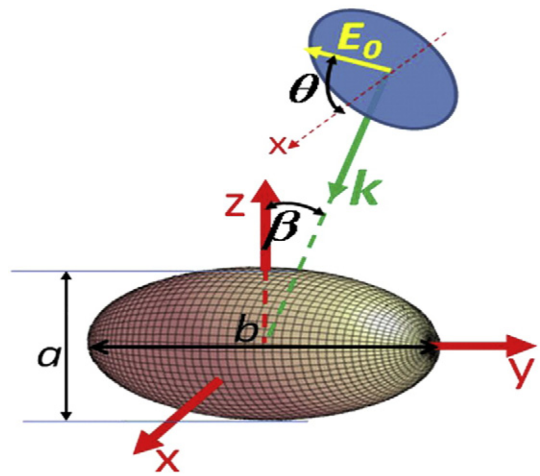

Fig. 2. Sketch of the silver nano-spheroid illuminated by linearly polarized light wave. The lengths of the major axis and the minor axis of the nano-spheroid are equal to b and a, respectively. The nano-spheroid is rotated symmetrical to y-axis. The incident angle β is defined as the angle from z-axis to the wave vector $\vec{k}$ of the illuminating light, and the polarization angle θ is defined as the angle from x-axis to the incident electric field $\vec{E_0}$.