Optics Communications 283 (2010) 2947–2952

Contents lists available at ScienceDirect

Optics Communications

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

Theoretical studies on the near field properties of non-concentric core–shell nanoparticle dimers

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ARTICLE INFO

Article history:
Received 7 December 2009
Received in revised form 1 March 2010
Accepted 15 March 2010

Keywords:
Nanoparticle
Dimer
Near field
Enhancement

ABSTRACT

The concentric core–shell nanoparticle dimers have "hot spots" with enhanced electric fields in their junctions, which can be used in the surface enhanced Raman spectra analysis. Here the non-concentric core–shell nanoparticle dimers are proposed by introducing a shift between the dielectric core and the metal shell. By using the three dimensional finite difference time domain method, the plasmon resonances and the near field properties of the core–shell nanoparticle dimers affected by the non-concentric shift, dimer separation, excitation wavelength and polarization are analyzed in detail. The results show that the local near fields of the non-concentric core–shell nanoparticle dimers can be much more enhanced than those of the concentric ones. Also the plasmon resonance wavelengths of the dimers can be effectively tuned by the non-concentric shifts between the core and shell. The proposed nanostructures can have great potential in various near field applications.

1. Introduction

The noble metallic nanoparticles have received particular research attention because of their capabilities of great local near field enhancements, which are due to the local surface plasmon (LSP) modes on the metal surface [1]. The optical properties of noble metallic nanoparticles with various shapes have been analyzed, including nanospheres [1], nanoprisms [2], nanorods [3], nanocubes [4], etc. And they have been used in many applications, such as surface enhanced Raman scattering (SERS) [3–5], surface enhanced fluorescence [6,7], chemical and biological sensors [8], nanoparticle waveguides [9], and optical nonlinear measurements [10]. Among these metal nanostructures, the metal nanosphere is the most popular and mature structure due to its easy fabrication process. Recently, the core–shell nanoparticle which is composed of a dielectric core surrounded by a metal shell has been studied because its plasmon resonance wavelengths can be tuned by varying the core size or shell thickness [11,12]. And the LSP modes of the nanoshells with a non-concentric core (termed as nanoegg) have been analyzed recently [13–15]. In the SERS applications, usually the aggregated core–shell nanoparticles are used and the random "hot spots" may be formed by the pair of closely spaced core–shell nanoparticles, which are termed as the dimers [5]. The "hot spots" are caused by the strong coupling interactions between the near fields of two closely spaced nanoparticles. In the fabrication process, both the concentric and non-concentric core–shell nanoparticles can be formed. Although the concentric core–shell nanoparticle dimers have already been analyzed [5,16], the non-concentric ones have not been analyzed yet.

In this article, the plasmon resonances and near field proprieties of the non-concentric core–shell nanoparticle dimers are analyzed in detail using the finite difference time domain method (FDTD). The simulation results show that the non-concentric core–shell nanoparticle dimers can also form the "hot spots" in their junctions like the concentric ones. Furthermore, the local near fields in the "hot spots" of the non-concentric core–shell nanoparticle dimers are much more enhanced than those of the concentric ones, which is essential for the near field applications. Also the plasmon resonance wavelengths of the dimers can be tuned by the non-concentric shifts between the cores and shells.

The organization of this paper is as follows. In Section 2, the three dimensional FDTD method used to model the nanoparticles is briefly introduced. In Section 3, the optical properties of the non-concentric core–shell nanoparticle dimers are analyzed in detail by the FDTD method. The influences of the dimer structure and the optical excitation parameters on the plasmon resonances as well as the local near fields are investigated. Finally, the conclusions are presented.

2. FDTD modeling method

The FDTD method is the most popular method to analyze the optical properties of the nanoparticles [11–23] and a homemade FDTD program is used in the simulations. The method is an explicit time-marching algorithm used to solve Maxwell's curl equations on a

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doi:10.1016/j.optcom.2010.03.033

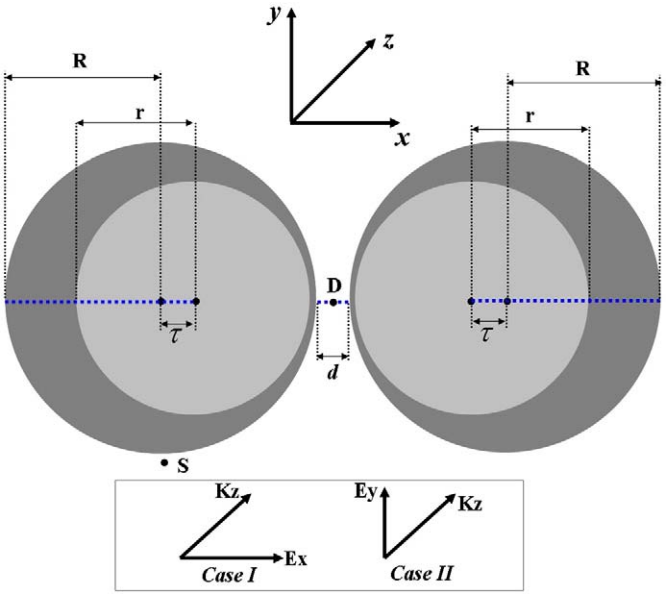

Fig. 1. The simulation schematic of the core–shell nanoparticle dimer.

discredited spatial grid termed as the "Yee cell" [22,23]. In order to model the dispersive metal material, the modified Debye model for the frequency-dependent permittivity function is used [21].

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} + \frac{\sigma}{i\omega\varepsilon_0} \tag{1}$$

Where ε is the complex relative permittivity of metal, ω is the angular frequency, ε_∞ is the infinite-frequency relative permittivity, ε_s is the static relative permittivity, τ is the relaxation time, σ is the conductivity, and ε_0 is the permittivity of free space. In this article, we choose the SiO_2 (with permittivity of $\varepsilon_d = 2.25$) and silver as the dielectric core and metal shell materials, respectively. And $\varepsilon_s = -9530.5$, $\varepsilon_\infty = 3.8344$, $\sigma = 1.1486 \times 107$ S/m, and $\tau = 7.35 \times 10^{15}$ s are chosen to model the broadband response in the wavelength range of 400–1200 nm. Using Eq. (1), these parameters (with no real physical means) are obtained by numerical fitting on the real metal permittivity, which is determined by the experiment data [21].

In order to obtain the broadband optical response of the non-concentric core–shell nanoparticle dimers, a modulated Gaussian plane wave with amplitude of 1 V/m with the frequency spectrum covering the 400–1200 nm wavelength range was directed to the dimers. While for the single wavelength excitation, a plane wave with the particular wavelength was directed to the dimers. The calculation

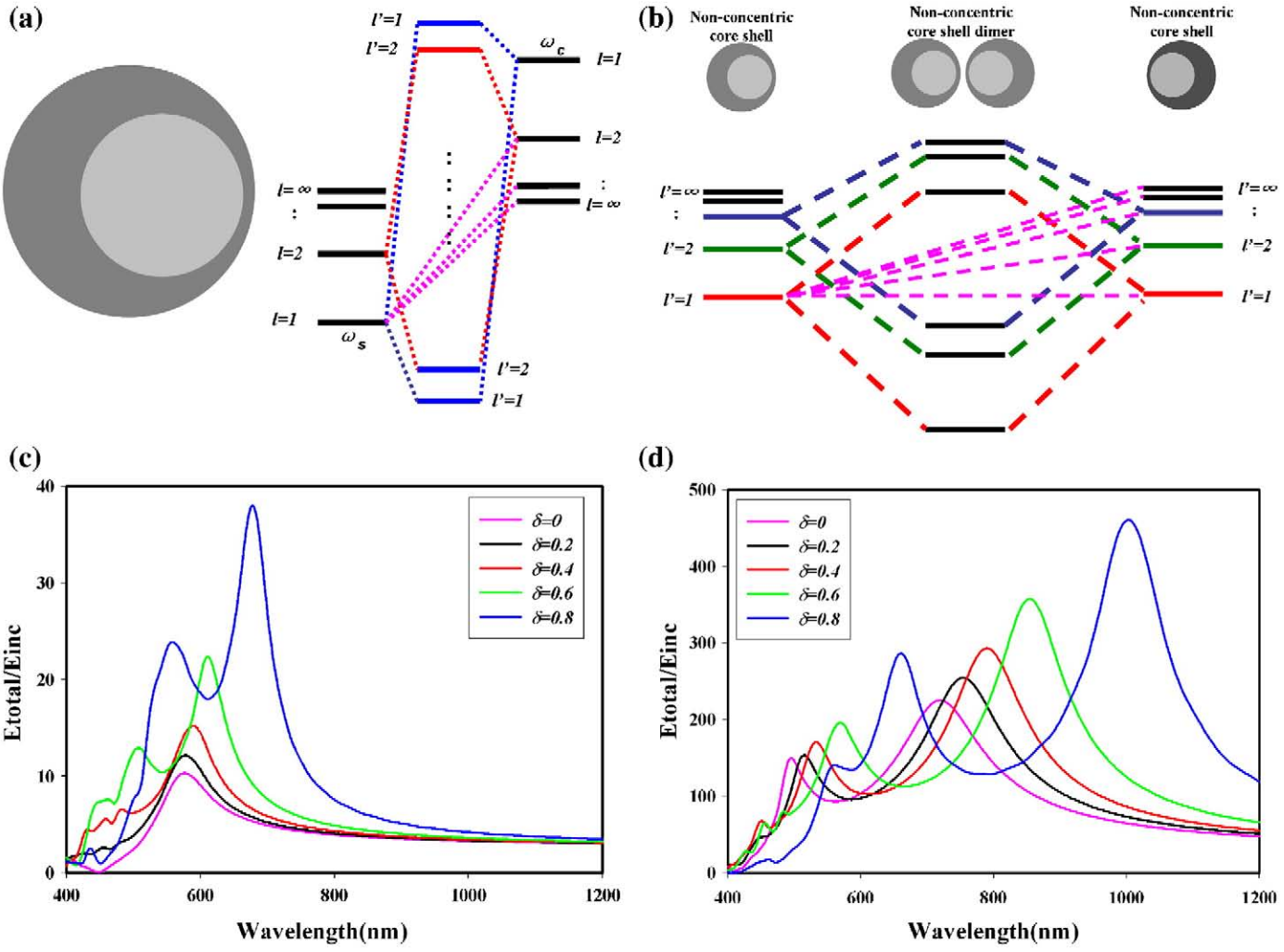

Fig. 2. (a) The energy level diagram for plasmon hybridization of single non-concentric core–shell particle; (b) the energy level diagram for plasmon hybridization of non-concentric core–shell dimer; (c) the near field enhancement spectra of single non-concentric core–shell particles with different δ; (d) the near field enhancement spectra of non-concentric core–shell dimers with different δ. (The gap size is $d = 2$ nm, polarization direction is parallel to the dimer axis).