Nanospheroidal particles as convenient nanoantenna elements

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A highly tunable optical nanoantenna element is proposed through gradual transformation from a sphere to a prolate spheroid. This new element induces field enhancement and an increase in resonance frequency. Rather than a purely metallic material, we propose the use of a metal-coated dielectric spheroid as a nanoelement because of its flexibility. We show that a spheroidal element enhances the near-field better than its rod and sphere counterparts. As such, spheroidal elements are good candidates for improving solar-cell performance.

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Guiding light through nanostructures is an important challenge for researchers today. A proper solution to issues related to this endeavor involves application of metallic nanoantennas[1−3]. Several schemes have taken advantage of the properties of localized optical near-fields generated by metallic nanoparticles; because of their unique activities, these nanoparticles are believed to have potential application in optical nanoantennas[4]. Antennas operating in the optical regime support localized surface plasmon resonance. Under certain conditions, light-excited plasmons lead to strong light scattering and absorption as well as enhancements of the local field. Plasmon modes exist in a number of geometries and in various metals, especially in noble metals such as gold and silver[5−6].

Research in the field of optical antennas is currently driven by the need for high-field enhancement, strong field localization, and large absorption cross-sections[7,8]. As an important application, high-field enhancement by optical antennas increases the light absorption efficiency of a device and yields specific improvements in solar-cell performance[9−12].

In this letter, we propose a highly tunable compact optical antenna obtained by introducing gradual changes in nanoparticle shape (from spherical to spheroid) to achieve high field enhancement. A second degree of adjustability is achieved by tuning the thickness of the metallic cover coating the dielectric core. The gradual change in shape from spherical to prolate spheroid is considered a primary step; this alteration in shape has interesting results. In the next step, the effect of cover thickness sweeping is considered after comparing pure metallic nanospheroids and metal-coated dielectric spheroids. The effects of different parameters on the resonance behavior of a single-element nanoantenna are further studied. Major and minor axis differences (ΔRs) and metallic cover thickness (h) are two important parameters to consider when designing nanoantennas; the current study focuses on variations in these two parameters. Since near-field enhancement is the main property described in this letter, the results may be applicable in future work on improving solar cells.

We briefly present important information about this work. Firstly, CST Microwave Studio (full-wave three-dimensional (3D) software) is applied as a main tool for the simulations, and a plane wave is used as incident light (E_{inc}) to excite the structure. Electric-field enhancement (E/E_{inc}) is a special near-field output; however, we also focus on the extinction cross section (ECS), which is a far-field output. In fact, the ECS is essential in studying parameter variations because its peaks occur at resonance frequency. By contrast, for direct ECS calculations, the broadband scattering response is extracted. Finally, the dielectric response of a noble metal modeled by the modified Debye model (MDM) must be determined.

In this letter, we investigate the properties of a single prolate nanospheroid as an improved nanoantenna element. Ellipsoidal particles with two principal axes of the same length are known as spheroids. Based on Fig. 1, rotation of the ellipse around the major axis generates a prolate spheroid (cigar-shaped).

In spheroids, we have an element resembling both a sphere and a rod featuring excellent properties when applied as an optical antenna. Such spheroidal particles are advantageous because they achieve strong near-field enhancements and provide a means of adjusting the scattering resonance frequency by changing the difference in the

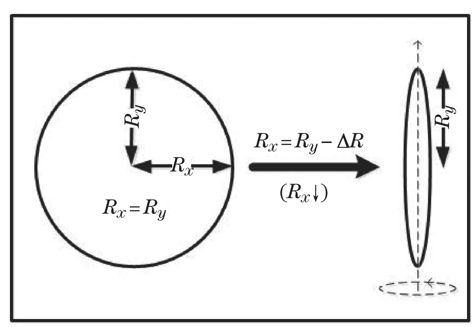

Fig. 1. Transformation from sphere to spheroid by ΔR sweeping.

axes (ΔR in shape). In addition to field enhancement, the resonance frequency of the proposed spheroidal element is nearly identical to that of a rod with a similar size. Thus, the effective wavelength of the spheroid is similar to that calculated for a rod element in a previous study[13]. This nanospheroidal element is a good replacement for both spheres and rods in nanoantenna arrays.

Based on the discussion above, we further investigate the proposed nanospheroidal element in this letter. To obtain substantial results, we modeled the dispersive behavior of a number of metals and selected an appropriate material for the experiments. Thus, before presenting the final simulation results, we provide a brief review of the results of dispersive modeling of two noble metals using the MDM over a broad frequency range.

Considering that the development of plasmonic structures as nanoantennas has become an important research topic, different numerical simulations have been used to design and optimize plasmonic structures. CST is a convenient software for this purpose. An important requirement of this software for the study of dispersive media is an analytical law of dispersion. While the Drude model may be used to describe metal dispersion at optical frequencies, the parameters of modeled materials must be applicable over broad frequency bands, to perform broadband calculations. Thus, in the this letter, MDM is used to describe the frequency-dependent behavior of metals; the constitutive parameters (ε, μ, σ, and τ) remain constant over a broad frequency band[14].

Since metals behave very differently in the optical domain[15,16], noble metals, such as gold and silver, are good candidates for optical antenna designs because these metals have specific optical properties. In this letter, we first model the metals in MATLAB and then load their results in CST. The complex relative permittivities of gold and silver calculated using MDM parameters over broad frequency bands are shown in Figs. 2(a) and 2(b), respectively. Silver was finally selected to construct the antenna because its permittivity, as described by MDM, covers a broader region of the frequency spectrum than gold.

We first show a scheme to improve the field enhancement in spheroids operating at the same resonance frequency (or effective wavelength) as rods. Then, we study the effects of gradual transformation of shape on the ECS by sweeping the ΔR parameter. We also focus on how field enhancements transform spheres into spheroids. Finally, after comparing field enhancements in a metal-coated silica element with that in a pure metallic element, how resonant frequency can be tuned by sweeping the h of the metallic layer is demonstrated.

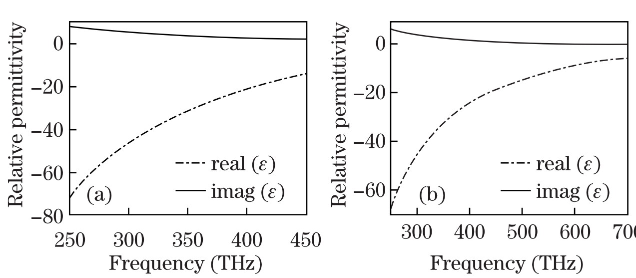

Fig. 2. Dispersive models of (a) gold and (b) silver based on the modified Debye model.

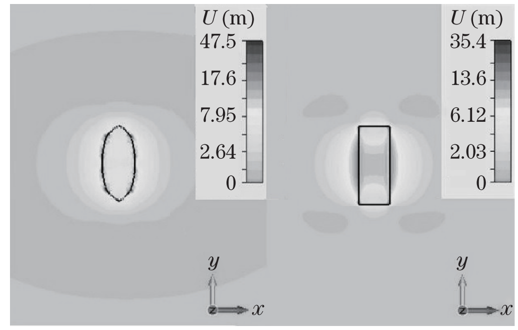

Fig. 3. Near-field enhancement of a prolate spheroid and a circular cylinder. Here, $l = 2 \times R_y$=100 nm, $\Delta R = 30$ nm, $R_x = R_y - \Delta R = 20$, and both particles are made from silver.

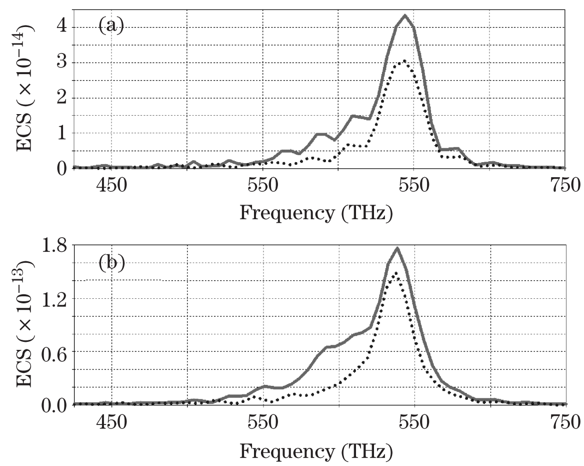

Fig. 4. ECS for both rod (solid lines) and prolate spheroid (dotted lines) with two different radii: (a) $R_x = 10$ nm; (b) $R_x = 20$ nm ($l = 2 \times R_y = 100$ nm, $\Delta R = 40$ and 30 nm in (a) and (b), respectively).

We model a prolate spheroid with dimensions of R_y (major axis) $\times R_x$ (minor axis) $\times R_x$, in which the fixed length (l) is equal to $2\times R_y$ and R_x changes from its maximum at the center to a minimum of zero at the tip end. Afterward, the near-field and ECS of this proposed model are compared with those of a cylinder with radius R_x (at maximum) and height l. Note that both elements are normally illuminated by a plane wave source and made from silver. Based on Fig. 3, the electrical field near the spheroidal nanoelement is considerably higher than the near-field around the cylindrical rod. However, the effective wavelength (or frequency) shows nearly no change in the proposed spheroid compared with that in the rod. This finding is confirmed by the ECS curves in Fig. 4. Prolate spheroidal nanoparticle can thus be considered suitable elements for use in optical antenna arrays for solar-cell applications.

A more complete study on the difference among axes is presented in this section. As shown in the diagram, a gradual increase in ΔR, as well as transformation from sphere to spheroid, causes a change in both resonance frequency and maximum amount of ECS. Based on Fig. 5, blue-shifts in resonance frequency are an important result of increasing ΔR.

As shown in Fig. 6, a gradual increase in ΔR and transformation from sphere to prolate spheroid causes strong field enhancements. Key dimensions of these two elements in nanospheroids are $R_y = 50$ nm and $\Delta R = 20$ nm. Thus, in terms of field enhancement, spheroids are more favorable than spheres as nanoantenna elements.

The appropriate combination of dielectric and metallic materials can produce highly tunable compact optical antenna. In fact, the resonant frequency can be tailored to operate over a wide range by properly controlling the cover thickness. Based on this principle, a concentric (core-shell) spheroidal nanoparticle composed of a plasmonic material (silver) and an ordinary dielectric material (silica) is examined here. This section gives new insights into the behavior of a two-layer nanospheroid and tunes its resonant frequency by means of the h.

The plot of ECS of a nanospheroid, in both pure metal (one layer) and core-shell model (two layers) forms, versus frequency is shown in Fig. 7. In the core-shell model, the core is made of silica with a permittivity of 2.08 and the silver shell has a thickness of 10 nm. The peaks occur at frequencies larger than 650 THz in the case of pure silver but at around 910 THz for silver-coated silica. Thus, based on the figure, the metal-coated dielectric material shows a considerable enhancement in resonance frequency. Figure 8 shows that the single-layer silver nanospheroid is capable of high near-field enhancements. However, silver-coated silica is a more favorable antenna material than pure silver because of the higher flexibility of the former compared with that of the latter.

As h is another important parameter to consider when building an optical antenna, we study the impact of increasing the h on the ECS. The calculated spectra clearly reflect the dependence of the two-layer nanoparticle ECS on h. Figure 9 shows that an increase in h causes a blue-shift in resonance frequency. Moreover, multi-resonance characteristics that may be utilized in several applications can be observed in the two-layer case. While the second resonance peak is not completely formed

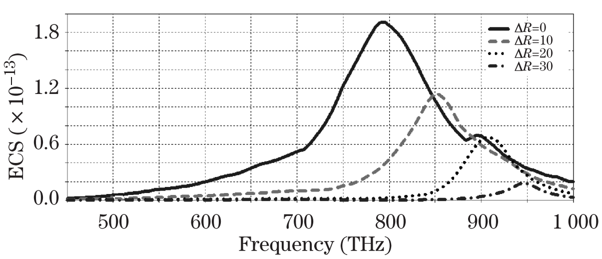

Fig. 5. Sweep ΔR for a silver nanospheroid (l = 100 nm, $\Delta R = 0 : 10 : 30$ nm).

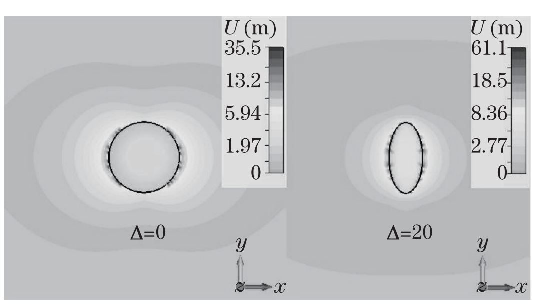

Fig. 6. Monitoring of the near-electric field in both spherical ($\Delta R = 0$) and spheroid ($\Delta R = 20$) nanoparticles ($R_y = 50$ nm).

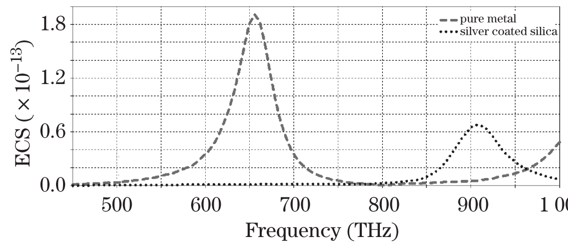

Fig. 7. ECS of a pure silver spheroid (dashed) and a silver-coated silica spheroid (dotted). For the external spheroid l_{ext}=100 nm, R_{x_ext} = 30 nm; for the internal spheroid $l_{\text{int}} = l_{\text{ext}} - h$, $R_{x\_\text{int}} = R_{x\_\text{ext}} - h$, and $h = 10$.

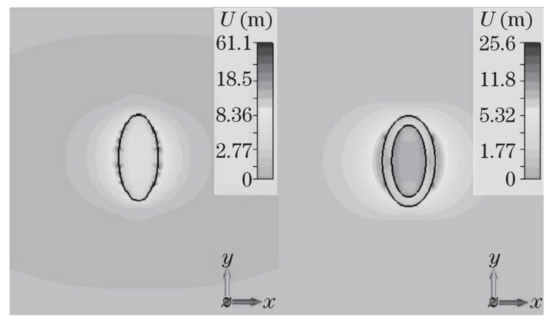

Fig. 8. Comparison of electric field enhancements in a pure metallic nanospheroid and a metal-coated dielectric spheroid (Dimensions are identical to those in Fig. 7).

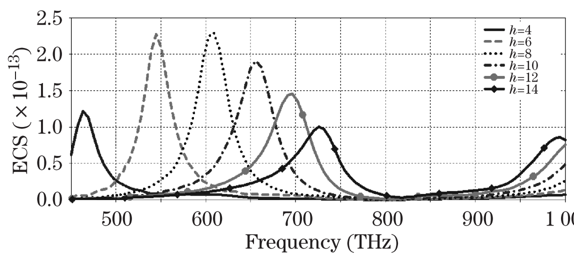

Fig. 9. Effect of cover thickness on the ECS of a silver-coated silica nanospheroid (l_{ext} = 100 nm, R_{x_ext} = 20 nm, and h=4:2:14).

in the frequency range under study, this peak remains observable. Gradual increases in h cause a blue-shift in the first peak and a red-shift in the second peak. This result serves as an additional tuning factor for achieving desirable optical properties.

In clusion, introduction of gradual alterations in nanoparticle shape from spherical to spheroid brings about an improvement in response. Thus, we obtained a semi-bar element with higher field enhancement but identical effective wavelength. Differences between the major and minor axes and h (in the metal-coated dielectric material) are two important parameters that control resonance responses. Nanoantenna arrays composed of nanospheroidal elements may be applied in various devices to improve solar-cell performance because of their ability to induce field enhancements.

References

1. L. Novotny, *Optical Antennas for Enhanced Light-Matter Interactions* (Report, The Institute of Optics, University

of Rochester, 2010).
2. P. Bharadwaj, B. Deutsch, and L. Novotny, Adv. Opt. Photon. **1**, 438 (2009).
3. P. Mühlschlegel, H. J. Eisler, O. J. F. Martin, B. Hecht, and D. W. Pohl, Science **308**, 1607 (2005).
4. M. L. Brongersma, Nature Photonics **2**, 270 (2008).
5. S. A. Maier, *Plasmonics: Fundamentals and Applications* (Springer, New York, 2007).
6. D. Guzatov and V. Klimov, New J. Phys. **13**, 053034 (2011).
7. L. Novotny, Phys. Today **64**, 47 (2011).
8. K. B. Crozier, A. Sundaramurthy, G. S. Kino, and C. F. Quate, J. Appl. Phys. **94**, 4632 (2003).
9. J. Li and N. Engheta, *IEEE Ant. Prop. Society Int. Symposium* 3388 (2007).
10. J. Xue, Q. Zhu, J. Liu, Y. Li, Z. Zhou, Z. Lin, J. Yan, J. Li, and X. Wang, Nanoscale Research Lett. **8**, 295 (2013).
11. K. Nakayama, K. Tanabe, and H. A. Atwater, Appl. Phys. Lett. **93**, 121904 (2008).
12. J. Zhao, G. Zheng, S. Li, H. Zhou, Y. Ma, R. Zhang, Y. Shi, and P. He, Chin. Opt. Lett. **10**, 042302 (2012).
13. L. Novotny, Phys. Rev. Lett. **98**, 266802 (2007).
14. H. Gai, J. Wang, and Q. Tian, Appl. Opt. **46**, 2229 (2007).
15. R. Thomas, J. Kumar, R. S. Swathi, and K. G. Thomas, Curr. Sci. **102**, 85 (2012).
16. M. A. Ordal, L. L. Long, R. J. Bell, S. E. Bell, R. R. Bell, R. W. Alexander, Jr., and C. A. Ward, Appl. Opt. **22**, 1099 (1983).