Numerical design of Au/Si core-shell nanoparticles

Larin A.O.1*, Sun Y. 1, Zuev D. A. 1

1Departure of Physics and Engineering, ITMO University, St. Petersburg 197101, Russia

*artem.larin@metalab.ifmo.ru

Abstract. Resonant metal-dielectric nanostructures of the core-shell type can provide unusual optical properties originated from spectral overlapping of electric and magnetic resonances of the nanostructure components. Here we numerically investigate the geometry and scattering cross section spectra of a core-shell nanostructure, where the core is gold, and the shell is crystalline silicon. We study spherical and cylindrical types of the nanostructures and search optimal geometrical parameters in the terms of spectral overlapping of the resonances. The obtained geometry parameters can be utilized for the first experimental realization of the metal-dielectric core-shell nanostructures.

1. Introduction.
Resonant plasmonics and dielectric nanoparticles have unique optical properties: surface enhancement Raman scattering [1], Kerker effect [2] and Fano resonance [3, 4], generation of high harmonics [5], etc. The unification of these types of nanoparticles in one structure gives combination of the properties of dielectric and metallic components as well as more freedom in obtaining of novel optical properties in such nanosystem [6].

In this paper, we present the results of analytical and numerical analysis of metal-dielectric nanoparticles with a core of gold and shell of silicon. Recently, the broadband unidirectional scattering was demonstrated theoretically in spherical metal-dielectric core shell nanoantenna [2]. Here, we examined the spherical as well as cylindrical shapes of the core-shell nanostructure to obtain spectral overlapping electric (ED) and magnetic (MD) dipole resonances of gold and silicon components respectively. The materials and size of cylindrical nanoantenna were set to obtain geometrical parameters which can be achieved by standard nanofabrication methods.

2. Results and discussion.
At first we have investigated the spherical core-shell nanoparticle. The description of the core is also similar to that one in problems for a homogeneous sphere in the field of an incident plane monochromatic wave; this method does not spend much time on the calculations. Scattering on spherical nanoparticles was modeled analytically by the Mie theory [7]. The field inside the core depends only on the first-order Bessel function. In the shell, the field is dependent on the Bessel functions of the first and second order [7]. Data on dielectric constants were taken from Ref. [8, 9]. We have investigated different values of the inner radius of the nanostructure in the range from 10 to
100 nm with the outer radius remaining constant of 150 nm. The simulation showed the dependence of the position and intensity of the scattering cross section of the electric dipole of a metal core on its internal radius. The spectrum was chosen, in which the point of the maximum value of the ED scattering cross section of the metal core corresponds to the value of the MD scattering cross section of the dielectric shell, in order to fulfill the first Kerker condition (figure 1). This is possible for inner and outer radius of the particle of 37.4 nm and 150 nm, respectively, at a wavelength of 1169 nm.

![Figure 1](image1.png)

**Figure 1.** Scattering cross section for a spherical core-shell nanoparticle in the air calculated on the basis of the Mie theory (shell radius of 150 nm, core radius of 37.4 nm). A dashed line designates the wavelength of the incident radiation at which unidirectional scattering is observed.

Developed model for a spherical nanoparticle were used to simulate a cylindrical structure, which can be fabricated by standard nanolithography techniques. To solve this problem, we used the FTDF method from the CST MicroWave studio. Features of geometry are the following: the half height of the cylinder corresponds to its radius, which was applied for both core and shell of the nanoparticle. This configuration maximizes the cylindrical shape to a spherical one. In addition, a plane monochromatic wave is directed along the axis of the cylinder, where the geometric cross section of the object gives a projection like that one for a spherical core-shell nanoparticle. The resulting spectrum of the scattering cross section for a designed cylindrical structure is shown on the figure 2.

![Figure 2](image2.png)

**Figure 2.** Scattering cross section for cylindrical core-shell nanoparticle in the air calculated on the basis of FTDT method (radius of a shell is 136 nm, radius of a core is 14.7 nm). The dashed line designates the wavelength of the incident radiation at which unidirectional scattering and azimuthally symmetry are observed. The inset shows the modeled structure and direction of propagation of the incident wave.
The size of the outer radius of the cylinder was chosen in such a way that the silicon nanoparticles of two types of the shape without core would have the same values of the resonant frequency for the MD resonance of the silicon. For this structure, the Kerker condition is satisfied at the wavelength of 1210 nm. The fulfillment of the Kerker condition is represented in the form of directional diagrams of the scattered light (figure 3). The smallest lobe beam width was obtained with an outer radius of cylinder of 136 nm and an inner one of 14.7 nm. The first figure (on the left side, figure 3) demonstrates the absence of backward scattering, the second (on the right side, figure 3) a presence of an azimuthally symmetry.

![Figure 3](image.png)

**Figure 3.** Scattering diagrams for a cylindrical core-shell nanoparticle: the diagram (on the left side) in the Oxz plane and (on the right side) in the Oxy plane. The coordinate system for the nanoparticle is indicated on the insets.

The carried out research demonstrates possibility of realization of unidirectional scattering in cylindrical hybrid nanostructure. The opportunity to adjust the optical properties is made by selecting materials for the core and shells, the particle size, and the relationship between the core and shell dimensions.

3. **Conclusion.**
In this work we have studied hybrid metal-dielectric core-shell nanoparticle to search conditions of resonances spectral overlapping (ED for gold core and MD for silicon shell) for unidirectional scattering realization. The geometry and material parameters were found for cylinder nanostructure which can be fabricated by existing nanolithography methods. The experimental realization of hybrid core-shell nanostructure and following experimental study of optical properties of such nanostructure can provide a set of interesting effects after the appropriate adaptation of the geometry of the structure and selection of materials: enhancement of Raman scattering, high order harmonic generation, etc. Moreover, application of silicon as a shell makes it possible to work with biological objects.

4. **Acknowledgments**
The Ministry of Education and Science of Russian Federation (Project 2.2267.2017/4.6) as well as Russian Foundation for Basic Research (Projects 17-02-00538, 16-29-05317). D. Zuev acknowledges the scholarship of the President of the Russian Federation.
References
[1] Jiangcai W and et. al. 2017 Surface Plasmon Resonance Sensors on Raman and Fluorescence Spectroscopy Sensors 17 2719 – 2730
[2] Liu W and et. al. 2012 Broadband Unidirectional Scattering by Magneto-Electric Core Shell Nanoparticles ACS Nano 6(6) 5489-5497
[3] Luk’yanchuk B and et.al. 2010 The Fano resonance in plasmonic nanostructures and metamaterials Nature Material 9 707 – 715
[4] Limonov M F and et.al. 2017 Fano resonances in photonics Materials 9 543 – 554
[5] Wang H and et.al. 2015 Janus magneto-electric nanosphere dimers exhibiting unidirectional visible light scattering and strong electromagnetic field enhancement ACS Nano 9(1) 436–448
[6] Toshihiko S and et al. 2017 Efficient third harmonic generation from metaldielectric hybrid nanoantennas Nano letters 17(4) 2647–2651
[7] Bohren C F and Huffman D R 1998 Absorption and Scattering of Light by Small Particles (Canada: A Wiley-Inter-science publication) A Potpourri of Particles: Coated sphere
[8] Johnson P B and Christy R W 1972 Optical Constants of the Noble Metals Phys. Rev. B 6 4370–4379
[9] Rakiand A D and et.al. 1998 Optical properties of metallic films for vertical-cavity optoelectronic devices Appl. Opt. 37 5271–5283