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Multipole optical response of silicon nanoparticles of a conical shape

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We explore the optical multipole resonances in silicon nanoparticles of a conical shape. We use the Finite Element Method (FEM) for solving the Maxwell equations for analysis of optical properties. Harnessing the multipole decomposition technique, we study excited optical resonances in silicon nanoparticles and the influence of high-order multipoles to scattering patterns of considered nanoparticles. Non-symmetrical combination of multipole contributions due to illumination from top and bottom sides of cones is also considered. Our work provides important information about the role of high order multipoles in the light scattering by non-spherical nanoparticles in the non-symmetrical case. Our results could be applied, for example, for development of metasurfaces and metamaterials in optical range, including asymmetrical ones.

1 INTRODUCTION

Optical properties of silicon nanoparticles attract great scientific interest [1–3]. These subwavelength scatterers can support the excitation of multipolar resonances [4] which enhance the light-matter interaction in a controlable manner just by changing the nanoparticles size, geometry and material [5,6]. It can be used for different applications, including nanoantennas [7, 8] and nanolenses [9, 10], cloaking [11,12], chemiluminescence microdevices [7] and composite plasmonic waveguide sensors [13,14]. Directional scattering induced by third order multipoles contribution in nanocylinders was recently investigated in [15]. A multipolar light-matter interaction has also been demonstrated by modifying properties of the illuminating radiation applied to a nano-scatterer with selective excitation of individual multipole modes in standing wave configurations [16]. Despite their intriguing properties and the theoretical progress in studying multipole resonances [5], their contribution to the scattering when they are excited in dielectrics of non-symmetrical shape is in fact omitted. To fulfill this gap in electromagnetic theory, we use finite element method in COMSOL Multiphysics and multipole decomposition technique [17] to study multipole resonances excited in silicon nanoparticles of conical geometries with varying height (H).

In contrast to previous works, where resonant dipole responses are usually considered in silicon nanostructures, here we pay attention to the higher order multipoles (up to the third order) and their role in the scattering pattern configuration.

2 RESULTS

Method of multipole decomposition of scattering cross-section was presented in [17] in details. Here we discuss this method briefly in general. Multipole moments in this method are calculated as integrals of different functions of induced displacement currents inside the nanoparticle volume. Next, using the irreducible representations of these multipoles, we can calculate contribution of each multipole into the total scattering cross-section. Multipole decomposition was recently implemented either for anapole mode investigations [18, 19] and for so-called super-dipole regime [15].

Below we introduce the following multipole moments: total electric dipole (TED) as sum of electric dipole and toroidal dipole moments; magnetic dipole (MD), electric quadrupole (EQ), magnetic

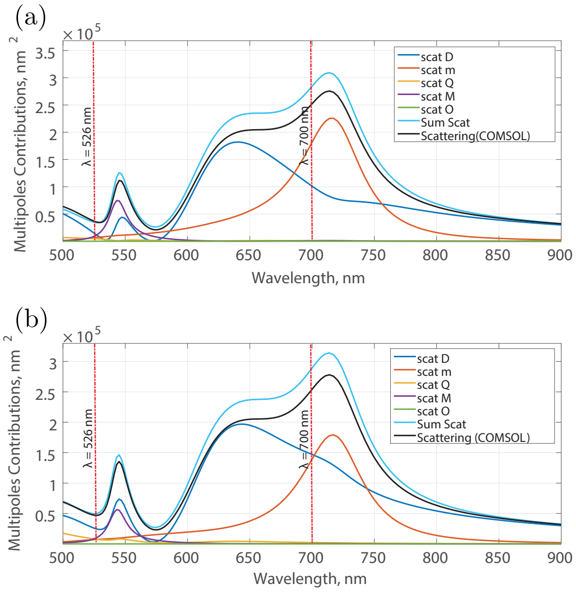

Figure 1: Multipole decomposition of nanocone scattering cross-section. Si nanocone, height $H = 250$ nm, diameter $D = 250$ nm. (a) Illumination from base side of the cone. (b) Illumination from top of the cone. Red dashed lines correspond to the spectrum points, for which scattering diagrams are considered below. Multipole contributions are contributions of corresponding multipoles to the total scattering cross-section of the particle, "Sum Scat" is the scattering cross-section as sum of multipole contributions, "Scattering (COMSOL)" is the scattering cross-section calculated directly with far-field integration.

quadrupole (MQ), electric octupole (OCT). We want to notice that taking into account only these first multipoles we describe optical properties of considered nanoparticles quite well.

2.1 Multipole analysis of conical nanoparticles' optical properties

Conical shape was chosen as quite simple for analysis, because it has a rotational symmetry, but with a strong geometrical anisotropy along its axis. So we expect to observe some asymmetrical peculiarities of scattering. They will be considered in the next section. In Fig. 1a we present a multipole decomposition for the conical nanoparticle with height $H = 250$ nm and base diameter $D = 250$ nm, illuminated from the base side; some special spectrum points designated with vertical dash-dotted red lines will be considered later.

In Fig. 2 we present the multipole behavior with respect to changing of conical particle height H. The second TED resonance disappears with the increasing of cone height (Fig. 2a), and the pronounced gap at the first resonance behaves similarly. In Figs. 2b–d we present the spectrum behavior of MD, EQ and MQ contributions to the scattering cross-section respectively for $H = 200$, 250 and 300 nm. EQ contribution is almost an order of magnitude smaller than another considered multipole contributions. One can note that EQ resonance (Fig. 2c) completely falls in the considered wavelength range only for $H = 300$ nm, but its behavior can be noticed for all heights for smaller wavelenghts. MD and MQ resonances (Figs. 2b, d) also shift to the red zone and rise as H increases. OCT contribution is much smaller than other and is not shown here because it does not affect the scattering features. In contradiction to, for instance, cubic particles [20], conical particles do not have separated scattering peak completely induced by MQ.

2.2 Asymmetry effect of scattering

Here, we consider influence of light incident direction at scattering process by conical nanoparticles. In this work, we consider nanoparticle with height $H = 250$ nm and base diameter $D = 250$ nm. It is important to study such processes due to possible difference between illumination from bottom and top sides. In Fig. 1 we show multipole decomposition spectra for (a) bottom side illumination and (b) top side illumination of silicon nanocone with height $H = 250$ nm and base edge $D = 250$ nm. One can note that although total scattering cross-section does not change crucially, multipole decomposition spectra are quite different. For the reversed illuminating (Fig. 1b), the electric moments TED and EQ provides larger contribution to the scattering cross section, and magnetic moments MD and MQ provides smaller contributions.

Different combinations of multipole contributions strongly influence scattering patterns. For instance, in Fig. 3 we consider 2D scattering patterns for conical nanoparticle at two wavelengths, corresponding to the big differences of multipole decomposition when changing the direction of light incidence. These wavelengths are marked in Fig. 1 with vertical dashed lines. In Figs. 3a, c we present scat-

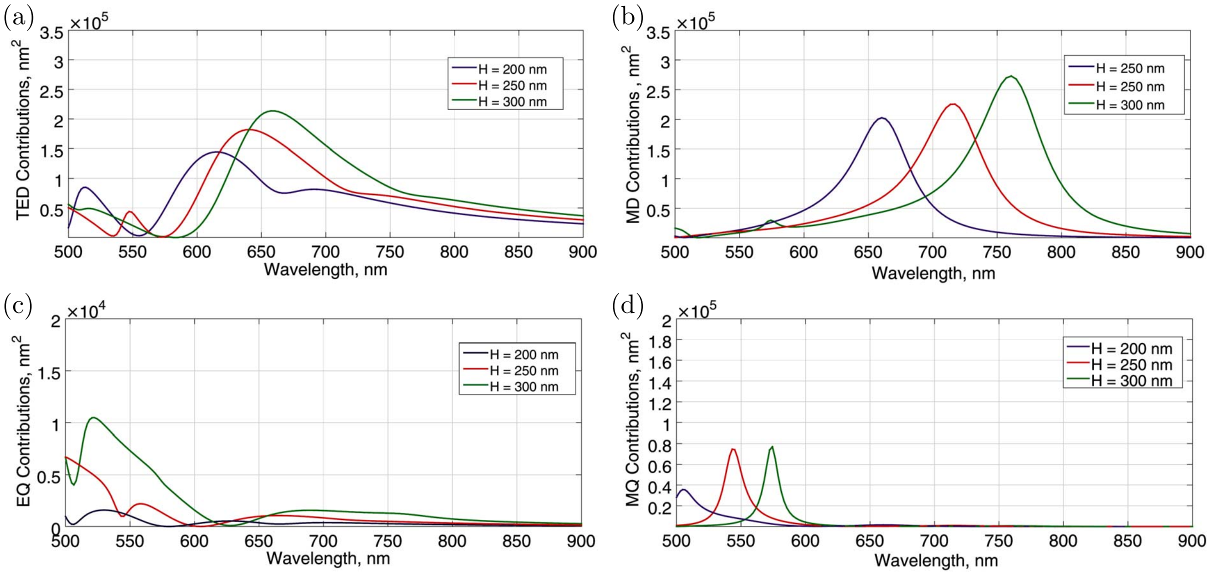

Figure 2: Multipole evolution in conical particles. All spectra are presented for Si nanocones with diameter $D = 250$ nm. (a) The TED spectrum for nanocones with $H = 200$, 250 and 300 nm. TED resonance for smaller wavelengths attenuates as H rises. The TED resonance in greater wavelengths has a gap for smaller H, and it becomes smoothed as H rises. (b) The MD spectrum for nanocones with $H = 200$, 250 and 300 nm. MD contribution increases and shifts to the red zone as H rises. (c) The EQ spectrum for nanocones with $H = 200$, 250 and 300 nm. EQ contribution increases and shifts to the red zone as H rises. It has a gap for for smaller H, and it becomes smoothed as H rises. (d) The MQ spectrum for nanocones with $H = 200$, 250 and 300 nm. MQ resonance increases and shifts to the red zone as H rises. Multipole contributions are contributions of corresponding multipoles to the total scattering cross-section of the particle ((a) TED, (b) MD, (c) EQ, (d) MQ.)

tering patterns for wavelength $\lambda = 526$ nm. As shown in Fig. 1, for this wavelength there is a specific point of all-multipoles lines crossing in the case of straight scattering (from base of the cone), what correspond to the side-scattering predominantly, and for reverse scattering (from top of the cone) scattering pattern correspond to the backscattering amplification with weaker side-scattering effect. In Figs. 3b,d one can see the results of TED and MD contributions interference for wavelength $\lambda = 700$ nm. For reversed illumination (Fig. 3d), Kerker conditions are almost fulfilled and very strong forward scattering suppression is observed. At the same time, for straight illumination backscattering almost does not attenuate for the same wavelength (Fig. 3b) because TED and MD contribution are very different.

These two spectrum points clearly show the existence of asymmetrical multipole responses in conical nanoparticles. The multipole decomposition for the reversed illumination is presented in Fig. 1b.

Asymmetry effect can be used for different applications, because it is triggered by illumination direction. Optical properties of the same object can be changed, although total scattering-cross section remains unchanged. Various bilateral metasurfaces and diodes can be developed using such effects.

3 CONCLUSION

We studied the multipole development as a function of the nano-scatterers height using the multipole decomposition method. We have considered the illumination of conical particles with different light direction and shown the effect of asymmetrical multipole responses in conical particles. Our work provides important information about the role of high order multipoles in the light scattering by non-spherical nanoparticles, including non-symmetrical cases. The results could be applicable, for example, for development of metasurfaces and metamaterials in optical range.

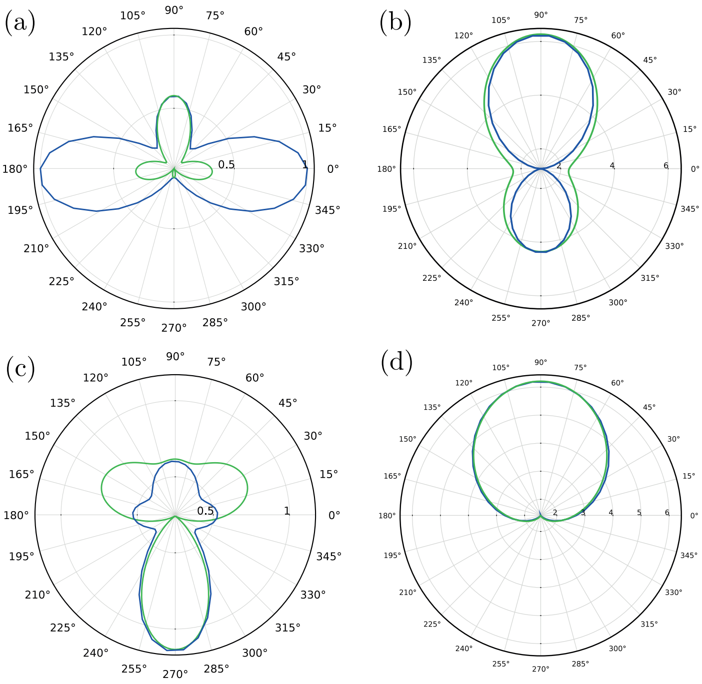

Figure 3: 2D Scattering patterns for two different directions of incident light. All patterns presented for the Si nanocone with height $H = 250$ nm and base edge $D = 250$ nm. (a) The straight incidence, $\lambda = 526$ nm. Approximately equal contributions of several multipoles provide side-scattering effect. (b) The straight incidence, $\lambda = 700$ nm. There is no Kerker-type effect at this wavelength, but only backscattering attenuation. (c) The reversed incidence, $\lambda = 526$ nm. Large TED contribution provides backscattering amplification and weaker side-scattering. (d) The reversed incidence, $\lambda = 700$ nm. Kerker-type effect can be noted. Blue (green) contour corresponds to the plane of the incident electric (magnetic) field polarization. Here forward/backward scattering direction corresponds to 90°/270°.

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