

تعیین خواص نوری نانوذرات مکعبی پلاسمونی با بکارگیری قطبش خارج از مرکز

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چکیده - در این مقاله یک روش نیمه تحلیلی و تقریبی اصلاح شده برای بدست آوردن ضریب قطبش‌پذیری و در نهایت پاسخ نوری نانوذره‌های مکعبی شکل برای قطبیدگی‌های مختلف پیشنهاد شده است. به جز کره، در سایر ذره‌ها ضریب دیپلاریزاسیون بشدت به موقعیت نقطه که معرف قطبش نقطه‌ای نانوذره در داخل حجم آن و بواسطه‌ی آن تعیین کننده پاسخ نوری در تقریب شبه‌ساکن است بستگی دارد. با استفاده از توزیع میدان نزدیک داخل نانوذرات مکعبی شکل، قطبش در نقاطی خارج از مرکز به عنوان نماینده قطبش الکتریکی کل ذره، مشخص می‌شوند. در واقع در این نقاط مقدار میدان الکتریکی، میانگین میدان کل و ضرایب دیپلاریزاسیون آن می‌توانند خواص نوری نانوذرات را با تقریب خوبی پیش‌بینی کنند. نشان داده می‌شود که برای نانوذرات در نظر گرفته شده در تابش با قطبیدگی عمودی نظر به وابستگی خیلی ضعیف قطبش الکتریکی متناظر با پاسخ نوری و منتهی از تشدید پلاسمونی نانوذره فلزی، قطبش در نقطه مرکزی نانوذره همچنان معرف مناسبی برای بدست آوردن خواص نوری می‌باشد. هرچند، در تابش با قطبیدگی موازی به محض اینکه ارتفاع نانوذره افزایش می‌یابد نقطه مناسب به سمت سطوح بالایی یا پایینی آن جابجا شده و آفست پیدا می‌کند. بنابراین، دو قطبی‌های نقطه‌ای قرار داده شده در نقاط خارج از مرکز می‌توانند با تقریب خوبی خواص نوری نانوذرات مکعبی شکل را پیش‌بینی کنند. این روش و تئوری اصلاحی را می‌توان به نانوذرات با شکل‌های نامنظم مختلف تعمیم داد.

کلید واژه- قطبیدگی، ضرایب دیپلاریزاسیون، شکل نامنظم، نانوذرات مکعب مستطیلی.

Determination of Optical Properties of Plasmonic Cuboid Nanoparticles Using Off-Center Polarizability

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Abstract- In the present paper a modified semi-analytical approximate method for determination of polarizability and ultimately optical properties of cuboid nanoparticles for different incident polarizations is suggested. Except sphere, in other particles depolarization factor strongly depends on the position of the point inside the particle. Each point represents an electric point-dipole, approximately defining the optical response of the nanoparticle in quasistatic regime. Using the near field distribution inside a cuboid nanoparticle the proper off-center point as representative of the whole shape is determined. Actually in this point electric field has a mean value and depolarization factors of it could predict the optical properties of nanoparticles properly. For perpendicular polarization because of the weak dependency of the electric polarizability to the considered dimensions, center point polarizability is still a good candidate for determination of the optical properties. However, as the height of cuboid increases the deserving point moves toward the top/down surface for parallel polarization. Interestingly, assigned the point-dipole at this off-center point can predict the optical properties of the considered plasmonic nanocuboid with a good approximation. This point-dependent (PD) MLWA technique could be generalized to different nanoparticles with an irregular shape.

Keywords: Polarizability, Depolarization factors, Irregular shape, Cuboid nanoparticles, PD-MLWA.

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1 Introduction

Despite of advanced progresses in the field of plasmonics and design novel nanostructures, information about the optical properties of nanoparticles such as absorption, scattering, and extinction cross section are the basic ingredients in this research area. Valuable information which extend the insight of the researcher and push them a big step forward for suggestion novel nanostructures. However, this data often obtained using numerical methods [1-5].

In addition to numerical methods, some researchers have followed semi-analytical approach by evaluating the static depolarization field at the center of the nanoparticle and modified long wavelength approximation (MLWA) [6-7]. Although in the sphere, the static and dynamic depolarization factors for determining the depolarization field inside the nanoparticle are constant, in other particles this factors are strongly depend on the position of the point inside the particle. Therefore considering different points, unlike polarizability factors are obtained. Besides polarizability, static depolarization factor is the essential term in the calculation of the electric field in the source region including an electric current source [8]. Therefore, closed form of this factor for special shapes has been obtained [8].

In the present paper, we follow the MLWA procedure with a new insight for determination of the static and dynamic depolarization factors. Different off-center points for the electric point-dipoles are approximately considered as an optical representative of the whole nanoparticle for each polarization. In these points the electric field has a mean value relative to the whole shape.

This article is structured as follow: the main formulae for calculation of the polarizability and the depolarization factors inside the cuboid are presented. Then, the appropriate points for determination of the optical properties of cuboid nanoparticles are investigated. In this way

polarizations parallel and perpendicular to the axis of the particles are considered. Different dimensions for the height and the cross section are assumed.

2 Modified Theory

Following the MLWA procedure, polarizability coefficient of a nanoparticle can be written as [7]:

$$\alpha = \frac{(\varepsilon_2 - \varepsilon_1)}{1 + (\varepsilon_2 - \varepsilon_1)[L - i \frac{k^3 V}{6\pi} - \frac{k^2 V}{4\pi} D]} \quad (1)$$

where ε_2 and ε_1 are the dielectric constant of the plasmonic (Au) nanoparticle and the surrounding medium respectively, L and D are the static and dynamic depolarization factors, and V is the particle volume. Hence as α calculates, the optical properties of the particle could be determined [7].

Considering a cuboid as schematically shown in Fig. 1(a), L and D along different directions can be written as [7,9]:

$$L_x = \frac{a}{2\pi} \int_{-h/2}^{h/2} \int_{-a/2}^{a/2} \frac{dydz}{(a^2 + y^2 + (z - z_0)^2)^{(3/2)}} \quad (2)$$

$$D_x = \frac{1}{2V} \int_{-h/2}^{h/2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \frac{(2x^2 + y^2 + (z - z_0)^2)}{(x^2 + y^2 + (z - z_0)^2)^{(3/2)}} dx dy dz \quad (3)$$

$$L_z = \frac{1}{4\pi} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \left[\sum_{i=1}^2 \frac{(h/2 + (-1)^i z_0)}{(x^2 + y^2 + (h/2 + (-1)^i z_0)^2)^{(3/2)}} \right] dx dy \quad (4)$$

$$D_z = \frac{1}{2V} \int_{-h/2}^{h/2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} \frac{(x^2 + y^2 + 2(z - z_0)^2)}{(x^2 + y^2 + (z - z_0)^2)^{(3/2)}} dx dy dz \quad (5)$$

Static and dynamic depolarization factors (L and D) defined as a result of depolarization field. Since the amount of depolarization field (E_d) varies generally with the position of point within the volume of the particle, thus L and D are nonconstant and change as E_d varies.

Although, up to now the center point of the particle has been considered as a representative of the whole shape, but it is shown that in the case

nanocuboid this loses its validity and off-center point should be considered.

3 RESULTS AND DISCUSSIONS

First of all in order to validate our results we calculate L_{xx} at plane yz ($x=0$) inside a cube centered at the origin and the side are at $\pm 1/2$ in the x , y , and z axis directions. The result is displayed in Fig. 1(b). It is in excellent agreement with the Fig. 1 of ref. [8].

In the next step the optical properties of nanocuboid in the case perpendicular polarization are explored. Nanocuboids with $a = 50\text{nm}$ and different lengths ($h = 80$ and 120nm) are considered. The numerical simulations are performed using the finite-integration technique (FIT) [10] and theoretical results are obtained using MLWA procedure by considering center point for obtaining the depolarization factors. The incident wave direction is indicated in the inset of Fig. 2. As Fig. 2 shows, increasing the

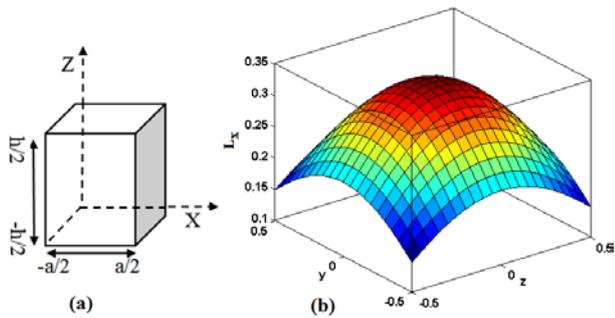


Fig. 1. a) A schematic view of the cuboid. b) L_x at yz plane of a cube with length 1.

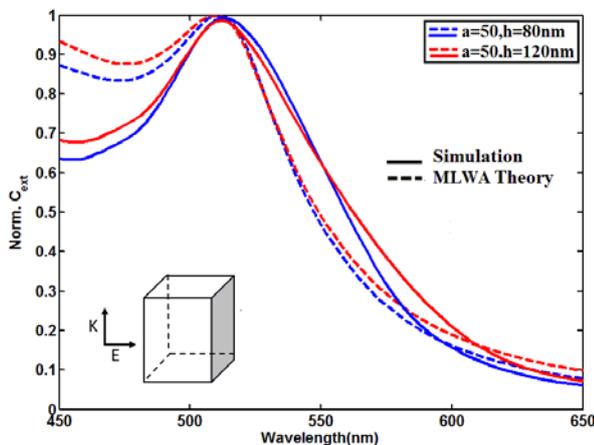


Fig. 2. Optical properties of nanocuboid with the $a = 50\text{ nm}$ and $h = 80$ and 120 nm . Electric field in along the x -axis. Solid and dashed lines show numerical and theoretical (MLWA) results respectively.

height of the particle has a negligible effect on the peak position of the LSP resonance mode. Moreover, while the electric field is parallel to the cross section of the particle, center point for the position of the point-dipole is a good candidate as an electromagnetic representative of the whole shape.

Furthermore, in order to see the validity of the center electric point dipole as a representative of the whole shape, the optical properties of nanocuboid with $a = 50\text{nm}$ and different lengths for parallel polarization are examined. The numerical and theoretical results for $h = 80, 120$, and 140 nm are shown in Fig. 3 (solid line and dashed line curves respectively).

Comparison between numerical and theoretical (MLWA) results show that there is a good agreement between the results for $h = 80\text{nm}$, however, as the length increases to $h = 140\text{nm}$ there is $\sim 140\text{nm}$ difference between them. Therefore as the length of the cuboid increases the center point of the particle loses its validity and could not properly predict the optical properties.

Actually, as the height of the particle increases the field becomes more non-uniform inside the particle and the field intensity increases at the top and bottom surfaces while it has a local minimum at the center of the particle. Following the near field distribution inside the particle reveals that depolarization factors at a point which the electric field has a mean value could predict the optical properties properly.

This appropriate point (P_z) for the point-dipole, is

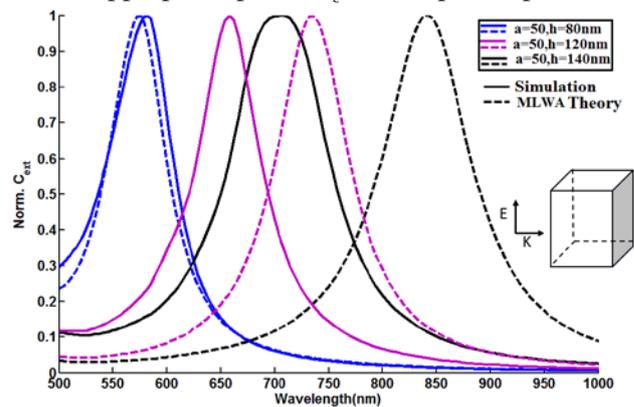


Fig. 3. Normalized extinction cross section of the nanocuboid with $a = 50\text{nm}$ and $h = 80, 120$, and 140 nm . Solid lines indicate the numerical results and dashed lines represent the MLWA results by considering center point. The inset shows the schematic view of the nanocuboid.

schematically shown in the inset of Fig. 4 for $h = 120$ and 140nm . As seen in Fig. 4, considering

P_z brings the LSP resonance mode to $\lambda=685\text{nm}$, while the numerical result represents the resonance mode at $\lambda=700\text{nm}$. Moreover, for $h=120\text{nm}$ results are exactly coincident. Consequently, good agreements between numerical results and modified theory, so-called the point dependent MLWA (PD-MLWA) technique, are achieved.

It should be added that as the width of the cuboid increases, the proper point for perpendicular polarization moves along the X axis toward the $X=\pm a/2$ plane a similar trend observed for parallel polarization.

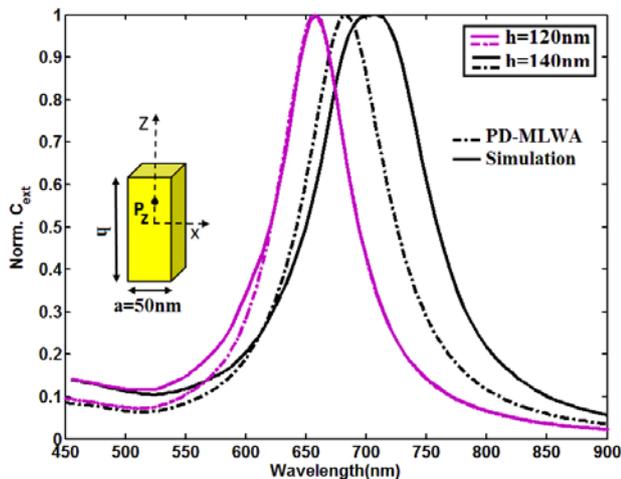


Fig. 4. Theoretical (PD-MLWA) and numerical results of the extinction cross section for the nanocuboid with $a = 50\text{nm}$ and $h = 120$ and 140nm . Theoretical result is obtained by considering P_z as schematically shown in the inset.

4 CONCLUSIONS

In summary, it has been shown in this paper that, as the depolarization factors strongly depend on the position of the point inside the particles, center electric point dipole is not usually the best candidate as a representative of the whole shape for obtaining the optical properties. Optical properties of nanocuboids for parallel and perpendicular polarizations have been investigated. As the height of the particle increases, the proper point for parallel polarization moves toward the top/bottom surface, while center point could predicts the optical properties in the case perpendicular polarization.

Therefore, our findings show that we can consider separate electric point dipole for each polarization inside a nanoparticle with an irregular shape. Knowing the appropriate points for each nanoparticle one can determines the polarizability. Accordingly, our study will open the door to novel plasmonic designs in a wide range of applications.

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