The 21St Iranian Conference on Optics & Photonics &
7th Iranian Conference On Photonics Engineering
13-15 January 2015, Shahid Beheshti University

توصیف خواص اپتیکی نانورینگ فلزی بر اساس نانوپوسته ی بیضی گون

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چکیده – خواص اپتیکی یک نانورینگ فلزی منفرد بر اساس تاثیر تغییرات ضخامت، شعاع داخلی و خارجی روی طیف سطح مقطع خاموشی مورد تحلیل قرار گرفته است. با ثابت در نظر گرفتن شعاع داخلی و ضخامت نانورینگ و تغییر شعاع خارجی، پدیده ی جدیدی در خواص اپتیکی مشاهده شده است. به طور دقیق تر، افزایش شعاع خارجی به ازای نسبت ابعاد (شعاع خارجی به ضخامت) کمتر از 3/2 منجر به تمایل به آبی در طیف خاموشی می شود، در حالیکه، به ازای نسبت ابعاد بیشتر از 3/2 تمایل به قرمز برای طول موج رزونانس پلاسمون سطحی محلی اتفاق می افتد. بعلاوه، با ثابت در نظر گرفتن شعاع خارجی و ضخامت، افزایش شعاع داخلی باعث تمایل به طول موج آبی در طیف خاموشی می گردد؛ در حالی که افزایش ضخامت باعث می شود نقاط بیشینه ی طیف خاموشی به طول موج آبی متمایل شوند. نشان داده شده است که خواص اپتیکی نانورینگ طلا می تواند بوسیله ی تئوری شبه استاتیک نانوپوسته های فلزی بیضی گون، توضیح داده شود؛ در حالی که، تئوری شناخته شده به عنوان مدل نانورینگ شبه ورقه نمی تواند این ویژگی را توجیه کند. نتایج شبیه سازی مدل تئوری پیشنهادی را تصدیق می کند.

کلید واژه- رزونانس پلاسمون سطحی محلی، سطح مقطع خاموشی، قابلیت قطبش، نانورینگ.

Spheroidal-Shaped Nanoshell Description for Optical Properties of Metallic Nanorings

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Abstract- *The optical properties of a single metallic nanoring (NR) have been analyzed according to variation of thickness, inner, and outer radius effects on the extinction cross section spectrum. It is shown that, by considering constant values for inner radius and thickness, a new phenomenon in optical properties is observed. More specifically, increasing the outer radius for the aspect ratio (i.e. outer radius/thickness) of less than 3.2, results in a blue-shift in the extinction spectrum, while for the aspect ratio of greater than 3.2 a red-shift for the LSPR (localized surface plasmon resonance) wavelength occurs. Moreover, by taking constant outer radius and thickness, increasing the inner radius results in a blue-shift for the extinction spectrum. Nonetheless, increasing the thickness leads to a blue-shift for the maximum peaks of the extinction spectrum. It has been shown that the optical properties for a gold NR can be described well through the quasi-static theory of a spheroidal shaped metallic nanoshell, while the previous theory for the NRs known as ‘‘slab like model’’ could not justify these properties. The analytic results supports the numerical simulations.*

Keywords*: Extinction, Localized Surface Plasmon Resonance, Nanoring, Polarizabilty.*

1 Introduction

The conduction band electrons of the noble metal nanoparticles can be excited under incident electromagnetic field. The curved surface of nanoparticles applies a restoration force to the driven electrons which results in a non-propagating collective electron charge oscillation known as Localized Surface Plasmon Resonance (LSPR) [1]. The nanoparticles show a large local field amplification in the near-field zone at resonance frequency. This unique property can be used in different applications such as chemical and biological sensors [2]. The LSPR wavelength is determined by nanoparticle shape, size, and surrounding dielectric constant [3]. A wide variety of nanoparticle structures are explored such as nanorings [4], nanoshells (NS) [5] and nanoholes [6]. The nanorings (NR) attracted remarkable attention which arises from the coupling of interior field to the environment [4]. The strength of electromagnetic coupling of the charge distribution of inner and outer NR walls, determine the LSPR energy and wavelength [7] similar to optical properties of a NS [8].

It has been shown that, the optical behavior of a nanodisk, can be modeled with an oblate spheroid [9]. Here, this idea is extended for modeling a gold NR with an oblate spheroidal NS composed of a gold spheroid shell surrounding a vacuum core.

2 Theory and Modeling

The well-known theoretical approaches for studying the optical properties of plasmonic nanostructures include: Mie theory (full wavelength analysis) and approximations such as quasi-static [10]. Due to the subwavelength nature of metallic nanoparticles, the quasi-static approximation can be applied to investigate the optical properties of metallic NRs.

A metallic nanoparticle response to an incident plane wave light (E_{inc}), can be modeled by a polarization vector described by [10]:

$$P = \alpha E_{inc} \quad (1)$$

where α is the electric polarizability of the NR which depends on the polarization direction of the incident wave.

It has been shown that the optical properties of an spherical nanoshell can be modeled using an electric dipole [11]. Using this idea, it is considered that the optical properties of a nanoring are modeled based on an oblate spheroidal shaped nanoshell. The electric polarizability of a spheroidal NS with ε_1 and ε_2 as inner and outer dielectric function and the volume of V, can be described using [10]:

$$\alpha_{NS}^{x}(\omega) = V\frac{(\varepsilon_2-\varepsilon_m)\left[\varepsilon_2+(\varepsilon_1-\varepsilon_2)(L_1-fL_2)\right]+f\varepsilon_2(\varepsilon_1-\varepsilon_2)}{\left[\varepsilon_2+(\varepsilon_1-\varepsilon_2)(L_1-fL_2)\right]\left[\varepsilon_m+(\varepsilon_2-\varepsilon_m)L_2\right]+fL_2\varepsilon_2(\varepsilon_1-\varepsilon_2)} \quad (2)$$

where $f = a_1b_1c_1 / a_2b_2c_2$ is the occupied volume fraction by the inner spheroid, $a_{1,2}$, $b_{1,2}$, $c_{1,2}$ are the axes of inner and outer spheroid respectively, L_1 and L_2 are the geometrical factors relating to inner and outer spheroids, respectively, which can be obtained by first and second kind of elliptic integrals. The modified long wavelength approximation (MLWA) correction term is employed in quasi-static approach [12]. Moreover, the dielectric function of gold material is described by Drude-Lorentz classical model with five poles [13].

The simulations are performed using finite difference time domain (FDTD) method using a commercial FDTD simulation software with the uniform mesh sizes of *dx= dy= dz=2 nm* and a 12-layer PML. The incident wave has a Gaussian frequency distribution from the wavelength 500 to 900 nm. Figure 1-a shows the schematic representation of the gold NR, and the incident plane wave is *x*-polarized. Furthermore, the *x*-polarized electric field of the NR (E_x) is recorded by the point monitor shown as *A* in Figure 1-a (situated on *x*-axis and 10 nm away from the NR edge).

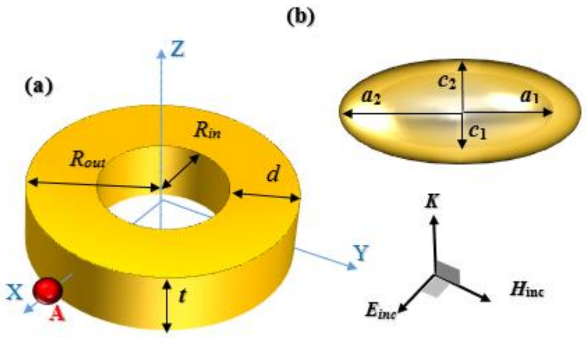

Figure 1: (a) The schematic representation of the gold NR. The point *A* is the near-field monitor point. (b) A simplified oblate spheroidal NS (b_1=a_1, and b_2=a_2 are the major axes).

3 Results and Discussions

Figure 2 shows the normalized amplitude of the electric field component E_x of the NR which is sampled at point *A* for a NR with $R_{in}=30$, $R_{out}=44$, $t=20$ *nm*. According to Figure 2, the theory using Equation 2 for an oblate NS ($\alpha_{NS}^{x}(\omega)$) with the major axes $a_1= b_1 = 35$, $a_2= b_2= 44$ *nm* and minor axes $c_1= c_2= 10$ *nm* (as the schematic NS depicted in Figure 2-b), is in complete agreement with the simulation results. The insets compare the spectrum of real and imaginary parts of $\alpha_{NS}^{x}(\omega)$ and E_x, respectively.

In addition, R_{in}, R_{out}, and *t* parameters are swept to analyze the dependency of extinction spectrum to geometrical parameters. Figure 3-a shows the extinction spectrum versus NR thickness. The results show a blue-shift pattern by increasing the NR thickness related to decreasing the electric field interaction between electric charges distributed on top and bottom NR surfaces. Figure 3-b shows the influence of inner radius increment on extinction spectrum. The inner radius changes from R_{in} = 15 nm to 30 nm results in an increase in the electric field interaction of inner and outer NR walls which leads to a red-shift in the LSPR wavelength. This structure is the geometrical complement of a void, created in a metallic medium, where increasing the void radius results in a similar red-shift in the extinction spectrum [1].

According to Figure 3-c, increasing the outer radius from aspect ratios (R_{out}/t) less than 3.2 results in a blue-shift of the extinction cross section spectrum and for the aspect ratios greater than 3.2 results in a red-shift. This property can be analyzed from the polarizability of the NS (Equation 2) in which setting the denominator of the polarizability predicts the position of the wavelength peaks. The latter property could not be described by the previous theories such as slab like model for the NRs[7].

To analyze the optical behavior of NRs during inner and outer radius variations, the simulated extinction peak wavelength are plotted versus the radius (Figure 4). The wavelength of the symmetric mode resonance, ω_{LSPR} (solid-line), for thin wall slab like NRs with a Drude dielectric model presented in [7] are shown. Figure 4-a shows the agreement of oblate spheroidal NS LSPR wavelength with simulated results of NR (marker) for different values of the inner radius. As it is depicted in Figure 4-a the slab like model could not describe the optical properties of the gold NR with the accuracy of the presented model. Figure 4-b also depicts the agreement of oblate spheroidal NS LSPR wavelength with simulated NR (marker) for different values of the outer radius.

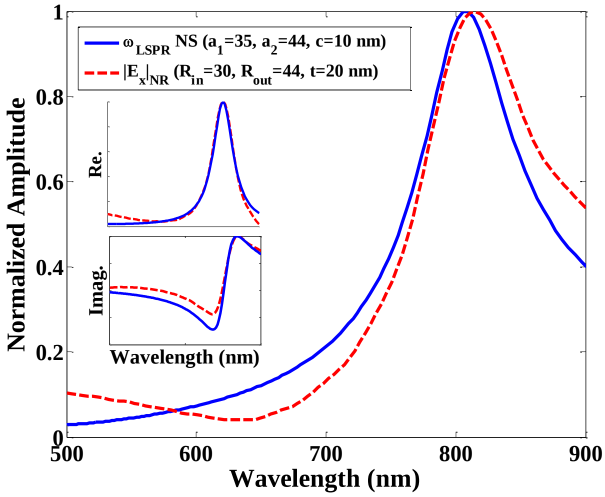

Figure 2: The absolute value of *x*-polarized electric field recorded by point monitor *A* of the NR (R_{in}=30, R_{out}=44, t=20 nm), being compared with an equivalent oblate spheroidal NS polarizability based on Equation 2 ($a_1=b_1=35$, $a_2=b_2=44$, $c_1=c_2=10$ nm). Insets show the real and imaginary parts of $\alpha_{NS}^{x}(\omega)$ and E_x.

The red-shift behavior observed for R_{out} > 64 nm (aspect ratios greater than 3.2) is similar to a conventional metallic nanodisk [12] which could not be described by slab like model.

4 Conclusion

To study the geometry dependence of localized surface plasmon resonance wavelength of nanorings (NRs), a gold NR immersed in vacuum with different thickness, inner and outer radii is analyzed. A novel optical behavior in high aspect ratio NRs is observed. It has been shown that the mentioned NR optical behavior can be explained by an oblate nanoshell with a gold shell surrounding a vacuum core.

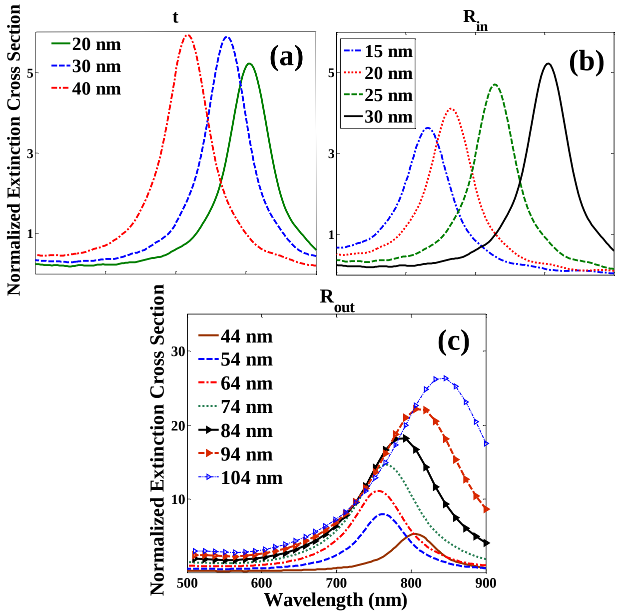

Figure 4: The normalized extinction cross section of the NR with variable thickness (a), inner radius (b) and variable outer radius (c).

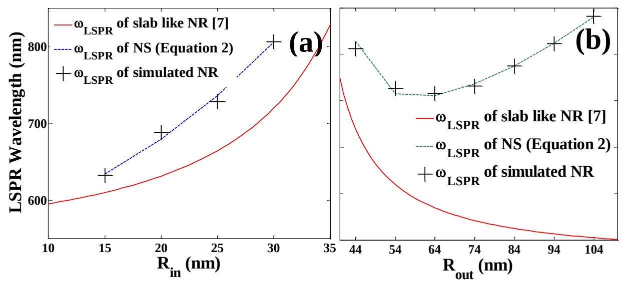

Figure 3: LSPR wavelength of a variable inner (a) and outer (b) radius simulated NR (marker) in complete agreement with an oblate spheroidal NS LSPR wavelength compared with symmetric mode wavelength of a slab like NR [7].

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