Absorption and Scattering Cross-Sections of the Spheroid Plasmon Nanoparticles

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Abstract—**This work is devoted to the study of the absorption and scattering cross-sections of the nonspherical plasmon nanoparticles. Influence of the dielectric permittivity of the surrounding media on the optical character of the non-symmetric nanoparticles has been researched.**

Index Terms—**nanoparticles; plasmon resonance; absorption and scattering cross-section**

I. Introduction

Metal nanoparticles are a separate class of the materials with unique properties, the study of which is of considerable scientific and practical value, due to the possibility of using such materials in all fields of science and technology, as active elements, such as sensors, photovoltaic devices, waveguides, filters, chemical catalysts, and other [1-5] The resonance of surface plasmons is the most pronounced optical property of metallic nanostructures, which manifests itself in the collective vibration of conduction electrons excited by the electromagnetic field of light.

It is necessary to distinguish the surface plasmons that are locked in the volume of metallic nanoparticles (the so-called first Fröhlich mode - dipole and multipole electron gas fluctuations near the surface of nanoparticles) and surface plasmon polaritons extending along the longitudinal boundary of the metal-dielectric and representing electromagnetic evanescent waves [6, 7]. More precisely, the surface plasmon resonance is a superposition of the electromagnetic waves and the polarization waves of the bounded by surface of the gas of free electrons. The conduction band electrons in the metal oscillate in resonance at certain wavelengths when light incidents on the metal nanostructure (size equal to or less than the wavelength of the incident light).

The surface plasmons are very sensitive to local changes in dielectric permittivity of the surrounding media since electromagnetic field is limited and localized on metal surface. Spectroscopy or detection of molecules is also possible due to the significant localization and amplification of the light field [8, 9].

Metal nanoparticles are of interest due to their unique electronic, optical and magnetic properties [10-12]. In particular, nanoparticles of noble metals such as gold and silver attract more attention, since they are characterized by a different color in the visible region in a result of plasmon resonance. The wavelength of the resonance strongly depends on the size and shape of the nanoparticles, the distance between the particles and the dielectric properties of the surrounding media [6, 13].

In most cases, spherical nanoparticles of the same size are considered [14, 15], but complex systems containing only identical stabilized nanoparticles are limited interest for technical and practical applications [16]. Isolated nanoparticles are of the highest interest for fundamental research, whereas for practical use systems with particles of different shapes and sizes that interact with each other are used. Therefore, the purposes of our work are the study of the optical characteristics of the nonspherical nanoparticles, namely, prolate and oblate spheroid nanoparticles; the study of their spectral characteristics, depending on the ratio between the semiaxes and the study of the effect of the dielectric permittivity of the surrounding media on their optical response.

II. Mathematical Background

In the general case, the frequency of plasmon resonance is determined by many factors, such as: the concentration and effective mass of conduction electrons, the shape, structure and particle size, the interaction between particles and the influence of the surrounding media. However, for an elementary description of optics of nanoparticles with plasmon resonance, a combination of the usual dipole approximation and the Drude theory is sufficient. In this case, the absorption and scattering of light by a small particle is determined by its electrostatic polarization α_0, which is calculated using optical dielectric permittivity $\varepsilon(\omega)$ or $\varepsilon(\lambda)$, where ω is the angular frequency, and λ is the wavelength in vacuum. For a small sphere of radius R in a homogeneous dielectric medium with dielectric permittivity ε_m, polarizability can be written as follows:

$$\alpha_0 = \frac{3V}{4\pi}\frac{\varepsilon_m - \varepsilon_h}{\varepsilon_m + 2\varepsilon_h} = R^3\frac{\varepsilon_m - \varepsilon_h}{\varepsilon_m + 2\varepsilon_h}, \quad (1)$$

and the cross section of absorption, scattering and extinction are equal:

$$C_{ext} = C_{abs} + C_{sca} = \\ = \frac{12\pi k\varepsilon_h \operatorname{Im}(\varepsilon_m)}{R^3|\varepsilon_m - \varepsilon_h|^2}|\alpha|^2 + \frac{8\pi}{3}k^4|\alpha|^2 \cong 4\pi k \operatorname{Im}(\alpha), \quad (2)$$

where $k = 2\pi\sqrt{\varepsilon_h}/\lambda$ is wave number of the medium.

Taking into account the renormalized effective Maxwell-Garnett theory [17], which takes into account the interaction between particles, one can write the renormalized averaged polarizability as follows:

$$\alpha^* = \frac{2\overline{\alpha}}{\kappa}\left\{1 - \frac{\sqrt{1-\kappa(1-\delta)}}{2}\left[\sqrt{1-\nu} + \frac{\arcsin(\nu^{1/2})}{\nu^{1/2}}\right]\right\}, \quad (3)$$

$$\overline{\alpha} = 1/3(2\alpha_\perp + \alpha_\parallel), \quad (4)$$

$$\kappa = f(\overline{\alpha}/R^3)^2, \quad (5)$$

$$\nu = 3\kappa\delta/(1-\kappa(1-\delta)), \quad (6)$$

The anisotropy parameter is equal to:

$$\delta = (\alpha_\perp - \alpha_\parallel)/(2\alpha_\perp + \alpha_\parallel), \quad (7)$$

Components of polarization tensor $\alpha_\perp$ and $\alpha_\parallel$ are equal:

$$\alpha_\perp = \frac{\varepsilon_m/\varepsilon_h - 1}{(\varepsilon_m/\varepsilon_h - 1)n_\perp + 1}\left(\frac{V}{4\pi}\right), \quad (8)$$

$$\alpha_\parallel = \frac{\varepsilon_m/\varepsilon_h - 1}{(\varepsilon_m/\varepsilon_h - 1)n_\parallel + 1}\left(\frac{V}{4\pi}\right), \quad (9)$$

where $n_\perp$ and $n_\parallel$ are geometric factors, which are called depolarization coefficients. For a spheroid with eccentricity e ($e \ll 1$):

$$n_\perp = \frac{1}{3} \mp \frac{1}{15}e^2, \quad (10)$$

$$n_\parallel = \frac{1}{3} \pm \frac{2}{15}e^2, \quad (11)$$

where the plus and minus signs correspond to the eccentricities in the vertical and horizontal directions of the spheroid.

III. Results and Discussions

Spheroid nanoparticles are selected as nonspherical nanoparticles. The silver was used as a material of nanoparticles with a refractive index from [18].

In the first step of our research was simulation of the absorption and scattering cross sections of the prolate spheroids when value of the transverse semiaxis changing from 10 to 40 nm for the fixed longitudinal semiaxis of 50 nm. The eccentricity varies from 0.2 to 0.8, respectively (see Fig. 1).

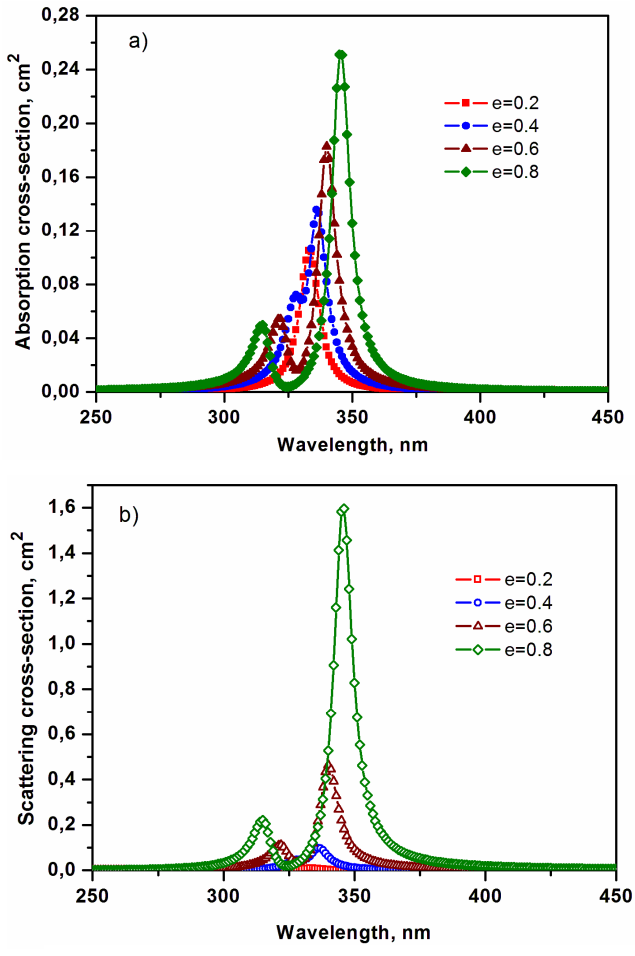

Figure 1. Dependences of the absorption and scattering cross-sections of the prolate spheroidal nanoparticles on wavelength at different eccentricities

As can be seen from Fig. 1 the maximum of absorption and scattering cross-sections are at the wavelength of 330 nm. An additional peak appears in the region of shorter wavelengths with an increase in eccentricity. The main peak is shifted to the region of longer wavelengths. Moreover, the distance between the peaks increases when eccentricity increases. In addition, the amplitude of the absorption cross section and the scattering cross section increases also. The absorption cross-section changes from 0.105 cm^2 (at the wavelength of 333 nm) to 0.251 cm^2 (at the wavelength of 345 nm). The scattering cross-section changes from 0.00919 cm^2 (at the wavelength of 333 nm) to 1.59 cm^2 (at the wavelength of 345 nm).

In case of the oblate spheroid nanoparticles, when value of the longitudinal semiaxis changing from 10 to 40 nm for the fixed transverse semiaxis of 50 nm, the additional peak appears in region of the longer wavelength (see fig. 2).

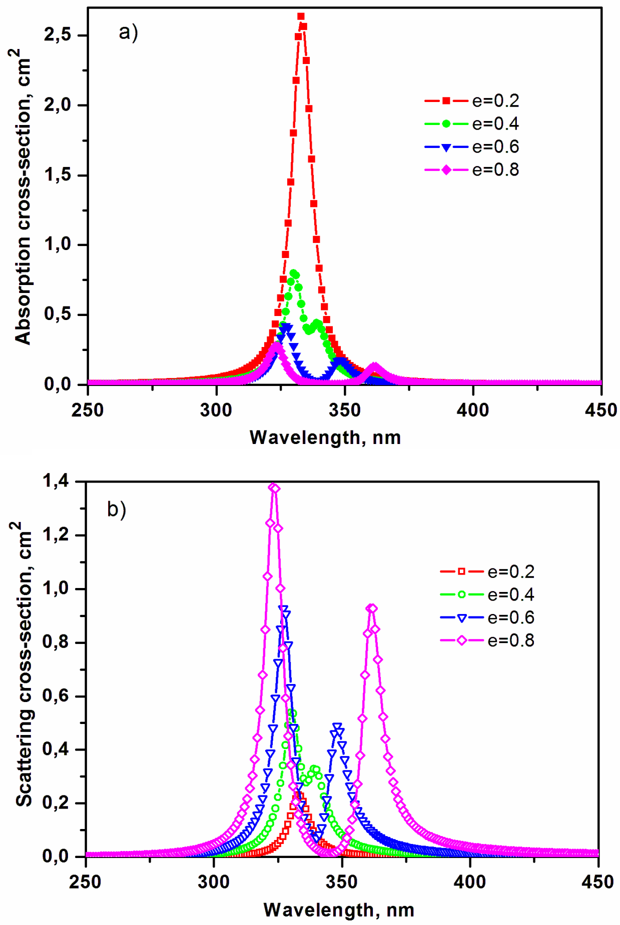

Figure 2. Dependences of the absorption and scattering cross-sections of the oblate spheroidal nanoparticles on wavelength at different eccentricities

Moreover, there is very interesting situation with absorption cross-section. Amplitude of the absorption cross-section of the oblate spheroid nanoparticles decreases when eccentricity increases. For example, maximum absorption is of 2.63 sm^2 (at the wavelength of 333 nm) for eccentricity of 0.2 and 0.277 sm^2 (at the wavelength of 323 nm) and 0.129 sm^2 (at the wavelength of 361 nm) for eccentricity of 0.8. It must be noted that distance between the peaks increases when eccentricity increases as for prolate spheroid nanoparticles.

In case scattering cross-section the additional peak appears in the region of longer wavelengths with the increase in eccentricity. The main peak is shifted to the region of the shorter wavelengths. The amplitude of the scattering cross section increases when eccentricity increased. The scattering cross-section changes from 0.23 cm^2 (at the wavelength of 333 nm) to 1.378 cm^2 (at the wavelength of 323 nm).

It should be noted that distance between peaks in case oblate spheroid nanoparticles is longer than in case prolate spheroid nanoparticles 38 nm and 31 nm respectively.

In the next step of our research the dependences of the absorption and scattering cross-sections of the prolate and oblate spheroid nanoparticles on wavelength at different refractive indices of the surrounding media were obtained (see Fig. 3 and Fig. 4).

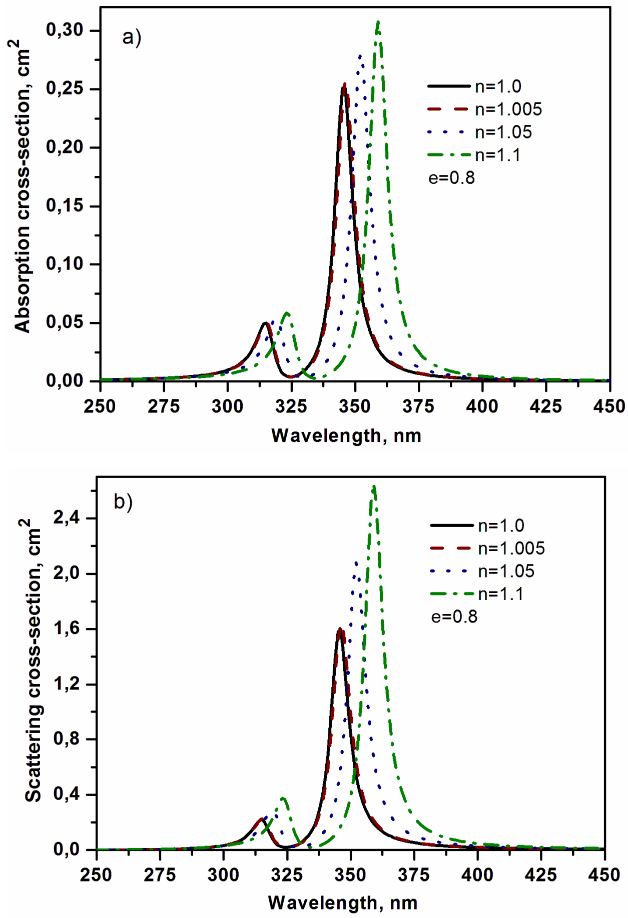

Figure 3. Dependences of the absorption and scattering cross-sections of the prolate spheroid nanoparticles on wavelength at different refractive indices of the surrounding media

The refractive index of the surrounding media was varied from 1.0 to 1.1. The spheroid nanoparticles with eccentricity of 0.8 were used for calculations.

The prolate and oblate spheroid nanoparticles demonstrate lower sensitivity to change of the refractive index of the surrounding media in third decimal place. Since spectral curves practically don't differ for refractive indices 1.0 and 1.005, as a result peak in at the wavelength of 315 nm for both type of spheroid nanoparticles.

Spectral curve of absorption cross-section shifts on 4 nm in case refractive index of 1.05 and on 8 nm in case refractive index of 1.05. The same results are demonstrated by the spectral curve of scattering cross-section.

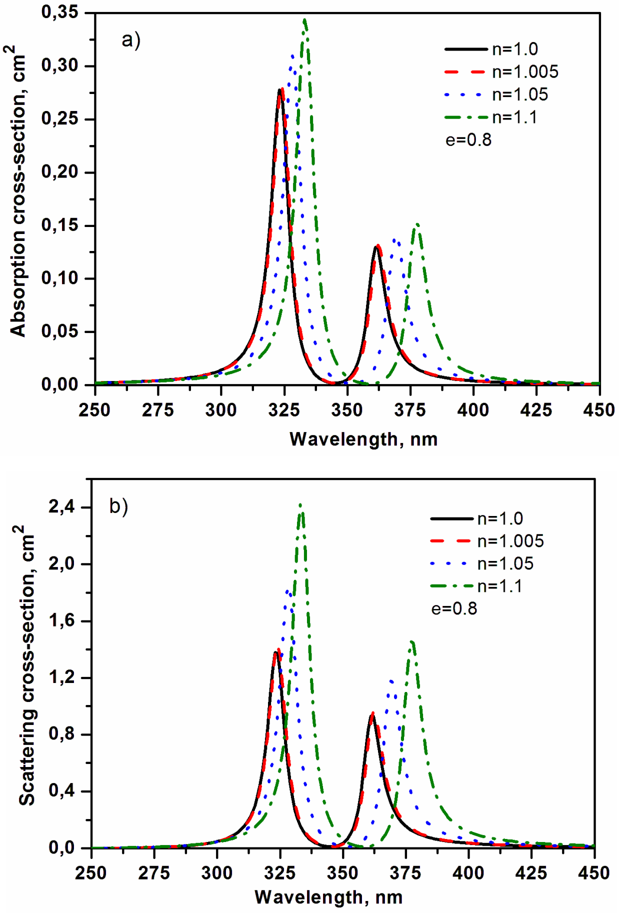

Figure 4. Dependences of the absorption and scattering cross-sections of the oblate spheroidal nanoparticles on wavelength at different refractive indices of the surrounding media

In case oblate nanoparticles spectral curves of absorption and scattering cross-sections also shift on 4 nm in case refractive index of 1.05 and on 8 nm in case refractive index of 1.05 from wavelength 324 nm to 328 nm and 332 nm respectively. In all cases resonance peaks are shifted to long wavelength region and amplitudes are increased when refractive index of the surrounding media increases.

IV. Conclusions

Simulation of the absorption and scattering cross-sections of the prolate and oblate spheroid plasmon nanoparticles on wavelength at different eccentricities was carried out. The additional peak appears in the region of shorter wavelengths with an increase in eccentricity in case prolate spheroid nanoparticles and additional peak with lower amplitude appears in the region of longer wavelengths with an increase in eccentricity in case oblate spheroid nanoparticles.

Influence of the dielectric permittivity of the surrounding media on the optical character of the spheroid nanoparticles has been researched. It is shown that resonance peaks are shifted to long wavelength region and amplitudes are increased when refractive index of the surrounding media increases. In generally we can conclude that prolate and oblate spheroid nanoparticles demonstrate the same sensitivity to change refractive indices of the surrounding media.

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