MODELING OF OPTICAL PROPERTIES OF HYBRID METAL-ORGANIC NANOSTRUCTURES

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I. INTRODUCTION

The development of modern nanotechnologies for the production of effective elements of nanophotonics, nanoplasmonics and nanoelectronics is largely aimed at the creation of hybrid nanostructures which include both plasmonic and organic components [1,2]. One of the types of such hybrid nanostructures are

ultradisperse media consisting of plasmonic metal-containing nanoparticles embedded in a matrix of organic semiconductors. With dense packing of nanoparticles in such nanocomposites, interparticle electrodynamic interactions associated with near-field scattering and coherent re-irradiation by particles of each other have the most important influence on their optical properties. By changing the material, size, shape or internal structure of plasmonic nanoparticles included in a hybrid metal-semiconductor nanocomposite, it is possible to adjust the degree of overlap of the spectral absorption bands of the nanocomposite components, which, in turn, affects the severity of near-field interparticle interactions. One of the ways to control the near-field scattering efficiency and absorption spectra characteristics of plasmon nanoparticles is to apply shells on their surfaces. This circumstance determines the importance of developing methods for modeling the optical properties of hybrid metal-organic nanostructures containing two-layer nanoparticles.

II. METHOD AND RESULTS

To model the spectral characteristics of such nanostructures, the extended Mie theory was used, which makes it possible to calculate the extinction efficiency factor (Q_{ext}) and the scattering efficiency factor in the near zone (Q_{NF}) of two-layer spherical particles placed in an absorbing matrix [3,4]:

$$Q_{ext} = \frac{4 m_i^2}{m_r \left[1 + e^{\eta}(\eta - 1)\right]} \, \mathrm{Re} \left\{ \frac{1}{m_i - im_r} \sum_{n=1}^{\infty} \left[(2n+1)\left(\psi_n^* \psi_n' - \psi_n \psi_n'^* + b_n \psi_n'^* \xi_n + b_n^* \psi_n \xi_n'^* - a_n \psi_n^* \xi_n' - a_n^* \psi_n' \xi_n^* \right) \right] \right\},$$

$$Q_{NF} = \frac{(4\pi m_i R)^2}{\lambda_0^2 \left[1 + e^{\eta}(\eta - 1)\right]} \sum_{n=1}^{\infty} \left\{ |a_n|^2 \left[(n+1)|h_{n-1}|^2 + n|h_{n+1}|^2 \right] + (2n+1)|b_n|^2 |h_n|^2 \right\}.$$

Here λ_0 – is the wavelength of the incident radiation, $m = m_r - im_i$ – complex refractive index of the matrix, a_n, b_n – Mie coefficients, a – particle radius, $\eta = 4\pi a m_i / \lambda_0$. Riccati-Bessel functions and their derivatives (ψ_n, ξ_n, ψ_n', ξ_n'), as the spherical Hankel function of the first kind of order h_n depend on the diffraction parameter $\rho = 2\pi a/\lambda_0$. In the case of two-layer spherical particles, the Mie coefficients are functions of the complex refractive indices of the nucleus and shell, the diffraction parameters of the particle as a whole and its nucleus.

The Q_{ext} value determines the attenuation of the intensity of the incident light beam caused by absorption in the particle and scattering on it. The Q_{NF} factor characterizes an increase in the intensity of the field along the surface of a sphere of radius R when nanoparticles are introduced into the center of this sphere.

Figures 1, 2 show the spectral dependences of Q_{ext} and Q_{NF} factors for two-layer plasmon nanospheres consisting of a metallic core (Ag, Cu) coated with a dielectric shell, placed in the organic semiconductor matrix of copper phthalocyanine (CuPc). The near-field scattering efficiency factor was calculated for R = R_2, where R_2 is an external radius of a two-layer nanosphere. As one can see, dielectric shell allows shifting the surface plasmon resonance band of plasmonic nanoparticles absorption both to short- and long-wavelength spectral range depending on the relation between shell and matrix refractive indexes. However, for cases under consideration, the appearance of dielectric shells on the plasmonic core leads to strong decrease of the Q_{ext} and Q_{NF} values.
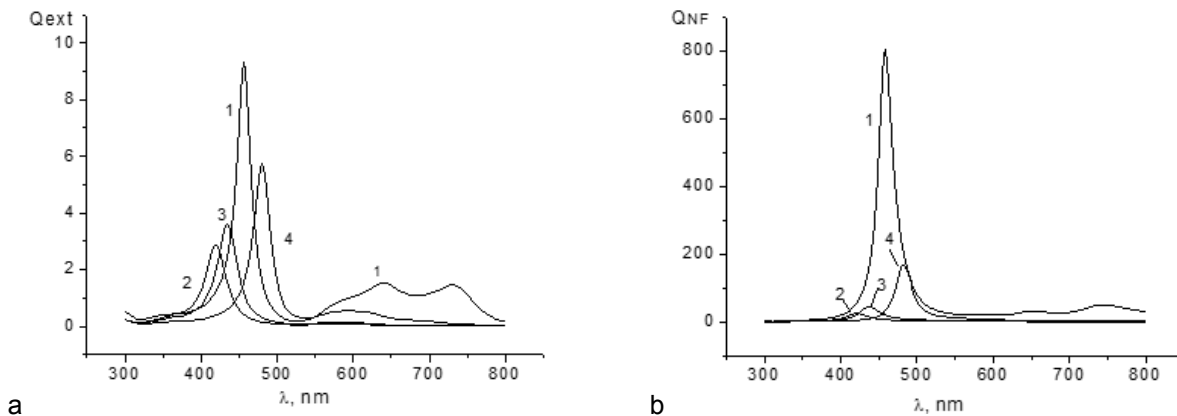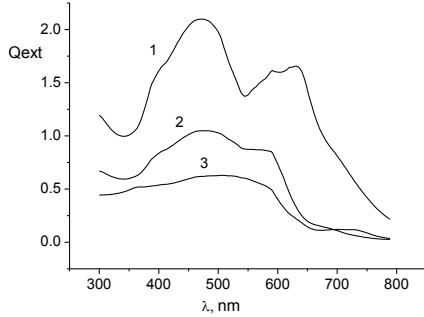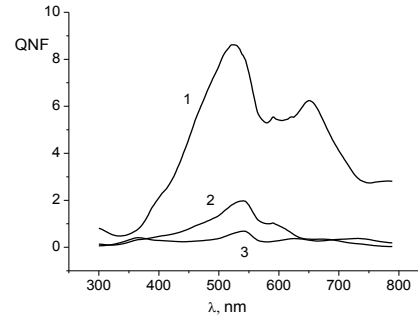

Figure 1. Spectral dependence of the extinction efficiency factor (a) and the near-field scattering efficiency factor (b) for silver nanoparticle (curve 1) and two-layer nanospheres with silver core and dielectric shell (curves 2-4) placed in the CuPc matrix. The radius of the silver core R_1 = 10 nm, the outer radius of the two-layer sphere R_2 = 15 nm. Refractive index of dielectric shell n =1.35, 1.5, 2.0 (curves 2, 3, 4 correspondingly)

a   b

Figure 2. Spectral dependence of the extinction efficiency factor (a) and the near-field scattering efficiency factor (b) for two-layer $Cu@SiO_2$ nanospheres placed in the CuPc matrix. The radius of the copper core R_1 = 25 nm, the outer radius of the two-layer sphere R_2 = 30 nm (curve 1), 40 nm (curve 2), 50 nm (curve 3)

III. CONCLUSIONS

Results of numerical simulations show that attenuation spectra of hybrid metal-organic nanostructures, as well as the near field effects at the spectral range of absorption bands of organic component, can be regulated by changing plasmonic nanoparticle material, their size or shell refractive index and thickness. Besides, the degree of near-field interactions with dense packaging can be regulated by the choice of the matrix in which the nanoparticles are placed.

ACKNOWLEGMENTS

REFERENCES

[1] Sergey Lepeshov, Alexander Krasnok, Pavel Belov, Andrey Miroshnichenko "Hybrid Nanophotonics", Physics Uspekhi, V. 188, № 11, p. 1137-1154, 2018 [in Russian].

[2] A. D. Zamkovets, E. I. Aksiment'eva, A. N. Ponyavina «Spectral manifestation of surface plasmon resonance in polyparaphenylene–silver nanostructures», Journal of Optical Technology, Vol. 78, Issue 2, pp. 84-87, 2011.

[3] I. W. Sudiarta, P. Chylek, "Mie scattering formalism for spherical particles embedded in an absorbing medium," J. Opt. Soc. Am. A 18, 1275–1278, 2001.

[4] R. A. Dunich, A. N. Ponyavina, V. V. Filippov, «Local field enhancement near spherical nanoparticles in absorbing media», J.Appl.Spectr., V.76, pp.705-710, 2009.