

**OPTICAL PROPERTIES OF THE WAVEGUIDES IN THE FORM
OF VARIOUS CONFIGURATIONS OF ARRAYS OF NANOPARTICLES,
SYNTHESIZED ON THE ELECTROSTATICALLY FUNCTIONALIZED SUBSTRATE**

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Optical properties of periodic structures consisting of gold and silver nanoparticles have attracted increasing interest due to their possible applications in optoelectronic devices. Such structures can be used for the resonant inductive transmission of energy of the plasmon excitation between the elements of nanosized computing devices, routers in nanoscale, in different types of nanosensors.

Such arrays of nanoparticles can be obtained by nanolithography. However, the least expensive way to obtain ordered structures, which doesn't require a local physical effects, based on the ability of nanoparticles to self-assembly in the process of random Brownian collisions in disperse systems with a liquid environment (hydrosol). In this system, the structural self-organization can be reached on the substrate. The particles must be adsorbed in a certain bounded region of the substrate, forming the required configuration of particles. It is important to emphasize that in this case, the waveguide consists of mono-resonant nanoparticles of spherical shape. Selective adsorption of nanoparticles can be achieved in various ways of functionalization of substrate.

In our research we propose an electrostatic method of functionalization of the dielectric substrate, based on the using of metal nanopatterns located on the back side of the substrate on which an electric potential is applied.

Under certain conditions, we can observe the selective deposition of metal nanoparticles into one-dimensional ordered structure. We defined the parameters of this system and investigated its optical properties. It is shown, that we may synthesize only nonequidistant single-track chains of particles. In addition, we can use templates of different configurations (Fig. 1).

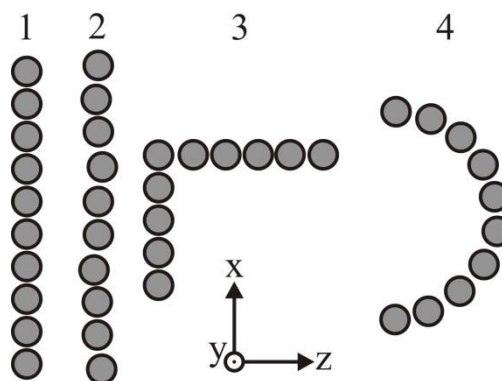


Figure 1 – Types of synthesized chains: 1) ideal chain; 2) real chain; 3) corner chain; 4) semicircle chain

The aim of the study is to determine the suitability of such configurations for transmission of optical radiation on the nanoscale by comparing their optical properties with optical properties of the ideal single-track and equidistant chains.

Calculations of the precipitation process of nanoparticles from the hydrosol satisfied by Brownian dynamics. At every iteration step, for each particle equations of motion (1) are solved:

$$\begin{cases} \frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i \\ m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i - \mathbf{F}_f + \mathbf{F}_c + \mathbf{F}_p + \mathbf{F}_d \end{cases}, \quad (1)$$

where \mathbf{r}_i , \mathbf{v}_i , m_i – coordinate, velocity and mass of the particle; \mathbf{F}_i – resultant of the potential forces acting on particle (van der Waals and elastic interaction, gravity force); \mathbf{F}_c – stochastic hydrodynamic force; \mathbf{F}_f – viscous force; \mathbf{F}_p – force that describes interaction with nanopattern; \mathbf{F}_d – force that describes dipole-dipole interaction between particles. We use predictor-corrector method to solve equations of motion (1).

Calculations of extinction spectra of synthesized chains are performed by the coupled dipole method. This method allows to calculate the absorption spectra of aggregates of closely spaced particles according to their electrodynamic interaction (any particle of aggregate in external optical field is influenced not only the external field, but the fields which generated by dipole moments, induced on the remaining particles). This electrodynamic interaction is the dominant factor that determines the non-uniform broadening of the plasmon absorption spectra. We solve a system of equations (2) to determine the dipole moments induced on the particles and to obtain the spectral dependence of the imaginary part of the optical susceptibility of the aggregate, which is determined by the absorption cross section (3).

$$d_{i\alpha} = \chi_0 \left[E_{\alpha}^{(0)} \exp(i\mathbf{k} \cdot \mathbf{r}_i) + \sum_{j=1, j \neq i}^N G_{\alpha\beta}(\mathbf{r}_{ij}) d_{j\beta} \right], \quad (2)$$

where $d_{i\alpha}$ – dipole moment induced on the given particle; χ_0 – polarizability of the particles; $E_{\alpha}^{(0)}$ – external optical field; $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$; $G_{\alpha\beta}(\mathbf{r}_{ij})$ – Green's tensor.

$$Q_e = \frac{\sigma_e}{N\pi R^2}, \quad (3)$$

where Q_e – extinction efficiency, σ_e – extinction cross-section, N – number of particles, R – radius of the particle.

We have calculated the extinction spectra of the synthesized chains of different configurations (Fig. 1) with different polarizations of the external optical field and for different values of interparticle gaps. In addition, we compared the spectra of synthesized chains with extinction spectra of ideal equidistant single-track chain. Chains, considered in this section, consist of $N = 10$ particles with $R = 8\text{nm}$ radius.

It is shown that the extinction spectra of real waveguide (Fig. 1(2)) slightly different from the extinction spectrum of an ideal chain (Fig. 2) in the case of longitudinal polarization of the external optical field (along the X axis). The extinction spectra of the real chain are shifted to shorter wavelengths, with increasing of the interparticle gap in the case of the same polarization of the external optical field. The extinction spectra of the ideal and real chains are almost identical when the polarization of the external radiation is directed along the Y axis (Fig. 2).

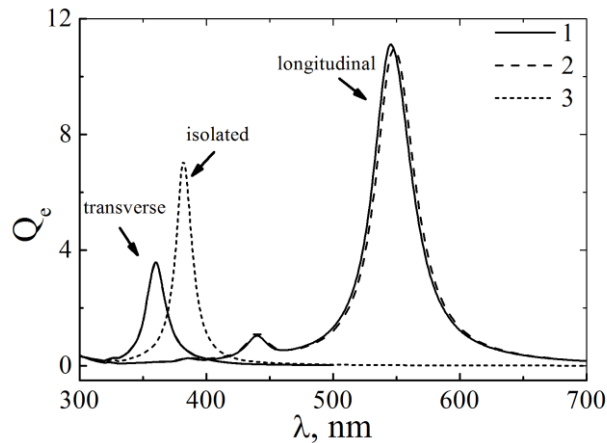


Figure 2 – extinction spectra of different chains with different polarization of external optical field (transverse – along Y axis, longitudinal – along X axis). 1) ideal chain; 2) real chain; 3) isolated particle

In addition, the extinction spectra of the corner chain (like the entire chain and its constituent parts, which are one-track chains directed along the axes X and Z) for different polarizations of the external optical field are calculated. It is shown that the extinction spectrum of the chain is the sum of the extinction spectra of its components when the polarization is directed along the X axis (Fig. 3). It is obvious that the transfer of plasmon excitation in the corner chain will be possible only if the polarization of the external radiation is directed orthogonally to the plane of the chain (along Y axis). In this case the maximum of the extinction of the whole chain and its constituent parts are practically identical (Fig. 3). Similar trend is also typical for the semicircle chain (data not shown).

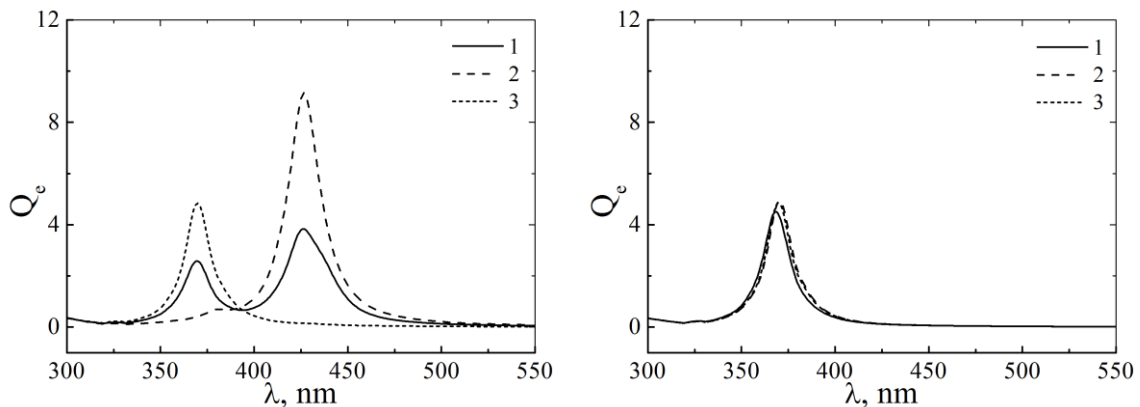


Figure 3 – extinction spectra of the corner chain and its constituent parts for polarization directed along X axis (left) and Y axis (right). 1) whole chain; 2) constituent part directed along X axis; 3) constituent part directed along Y axis

We have considered the extinction spectra of optical waveguides of different configurations consisting of chains of nanoparticles. It is shown that the extinction spectra of the synthesized in the experiment nonequidistant chains slightly different from the extinction spectrum of an ideal chain. This property gives the opportunity to use such system of closely spaced metal nanoparticles for transmission of electromagnetic energy at the nanoscale distances.