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Theoretical Modeling of Liquid Crystal Based Tunable Metamaterials

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SCIENCE AND TECHNOLOGY CENTER IN UKRAINE

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In the project, we propose to incorporate liquid crystals (LCs) into structures containing metamaterials (MMs), as one possible way of solving the challenging problem of their optical tunability. The objectives of the project are to develop the physics background and mathematical techniques enabling the evaluation of the effective electromagnetic parameters of the LC based metamaterials and study the possibility of tuning their optical properties. Configurations studied include MMs with nanoparticles or nanowires of core-shell type placed in isotropic/anisotropic (LC) matrix, layered structures of 2D conducting materials with dielectric (LC) layers, or structures with LC/metallic nanostrip grating/dielectric configurations. We predict the complex dielectric function, effective permittivity tensors, and optical properties of several configurations of these systems and demonstrate tunability by changing parameters of the system.

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Final Report

Theoretical Modeling of Liquid Crystal Based Tunable Metamaterials

STCU Project P521 (EOARD Grant #11-8007)

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Executive Summary

Project is directed on research of new structures containing metamaterials (MMs), which interact with incident electromagnetic waves and possess an optical tunability. MMs have inspired a series of significant technological developments and research giving flexibility in manipulating the electromagnetic waves and obtaining new functional materials, including the cloak of invisibility [1-11]. The interaction of MMs with electromagnetic waves can be accompanied by excitation of surface plasmons (SP) inside of MMs. Over the last decade, hyperbolic metamaterials (HMMs) have gained a central role. HMMs are uniaxial structures that combine the properties of transparent dielectrics and reflective metals. The effective permittivity tensor of HMMs has principal components of different signs. It results in appearing many new physical effects and applications [12-21]. Although the successful development of MMs has already been demonstrated, the next step in this very fast developing area of the modern physics and technique is required: to make MMs tunable and adaptive. Tunable and adaptive materials can dynamically optimize themselves to fit their current operating environment. The tuning ability helps to make metamaterial devices more versatile, adapting to shifting input or changing target parameters.

In the project, we propose to incorporate liquid crystals (LCs) into structures containing MMs, as one possible way of solving the challenging problem of their optical tunability. The main feature of LCs is ability to change physical properties considerably under small external fields. It allows to tune optical properties of these structures. The objectives of the project are to develop the physics background and mathematical techniques enabling the evaluation of the effective electromagnetic parameters of the LC based metamaterials and study the possibility of tuning their optical properties. Such MMs can contain nano-particles or nano-wires of core-shell type placed in isotropic/anisotropic (LC) matrix. They can also represent the layered structures of 2D conducting materials with dielectric (LC) layers or structures of type "LC - metallic nanostrip grating - dielectric".

We selected approaches and analytical expressions, which allow describing dielectric function of nano-particles in the area of localized SP resonance. For the core-shell nanoparticles with Au-core, we studied dependence of real and imaginary parts of their dielectric function on wavelength in the cases of homogeneous isotropic and anisotropic permittivity of the nano-particles shell. The light absorption by nanoparticles of different size with Au-core in the area of the plasmon resonance was calculated and analysed. Impact of nonlocality of dielectric function on optical response of metallic nanoparticles was considered. Using Maxwell-Garnet formalism the dielectric function of ensemble of spherical core-shell nanoparticles with Au-core was studied. It was shown that core-shell metal-dielectric nano-particles provide opportunity to tune the plasmon resonance frequency by changing properties of both core and shell. Adaptive core and/or shell may change their thickness and permittivity under the action of external stimuli that finally results in shift of the plasmon frequency and change of absorption and scattering cross sections.

Electric response of the objects covered by spherical and cylindrical shells with anisotropic permittivity is studied under the quasi-static uniform electric field. The shells permittivity components are radially power-law dependent on the distance to the shell center. We show that such shells can be used as invisibility cloak if radial and tangential components of the shell permittivity satisfy a certain relation between them. Efficiency of cloaking is studied and conditions for ideal cloaking are established. We obtained conditions allowing to reach the effective cloaking if the shell permittivity is isotropic. We studied the electrostatic responses of the cylindrical structures with magneto-optic core under steady uniform magnetic field. It was shown that cylindrical shells with anisotropic radially dependent permittivity can be used for cloaking of magneto-optic inclusions in magnetic field. Using a theory of space-time transformation and approach of generating function we considered several types of this function and calculated the corresponding radial dependence of the shell permittivity components. It gives a possibility to make easier a choosing of the shell permittivity radial dependence, necessary for practical realization of the invisibility cloak.

System of cylindrical core-shell nanowires periodically arranged with the sub-wavelength separation in isotropic/anisotropic dielectric matrix is studied. The effective permittivity tensor of the system is calculated in general case of radially power-law dependent components of the shell permittivity. For system of nanowires with the Au-core and Ag-core we obtained the frequency areas where the system has properties of HMM. Replacing isotropic dielectric matrix by anisotropic one allows to widen the HMM frequency area in the case of the Ag-core and obtain new HMM frequency areas in the case of the Au-core. Using as anisotropic matrix the LC 5CB and E7 we show that HMM areas are sensitive to the LC orientational state. Possibility to tune the position and wide of the HMM frequency areas by changing the parameters of nanowire or isotropic/anisotropic (LC) matrix is demonstrated.

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Light transmittance and reflectance of the three-layer system, isotropic dielectric – the paired gold nanowires grating – VO_2, is studied. We observe the minima/maxima in transmission/reflection spectra of the system, which are identified with the SPs excitation in the gold nanowires. Our modeling shows that we can effectively change transmittance/reflectance of the system on the SP resonance frequency by varying temperature from below to above the transition temperature semiconductor-metal in VO_2. Replacing VO_2 by the LC layer we show that the spectra of the system can be tuned by reorienting the LC director. Impact of the LC orientational state on the absorption spectra in the systems LC - MoS_2 micro-ribbon grating – Si and LC – graphene-MoS_2 micro-ribbon grating – Si is studied. The results suggest that control of the LC orientational state enables us to manipulate the absorption maxima corresponding to the SP excitation in the MoS_2 and the graphene-MoS_2 micro-ribbons. We considered a nanorod-mediated SP resonance sensor, which includes a glass prism, the LC layer, a thin metal film, a layer of aligned nanorods array, and a sensing layer. We studied the reflectance of the system in the area of the SP resonance and show that sensitivity of the system is controlled the LC orientational state.

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Project Objectives

Metamaterials are materials with electromagnetic properties that originate from man-made sub-wavelength structures. Metamaterials have inspired a series of significant technological developments and research giving flexibility in manipulating the electromagnetic waves and obtaining new functional materials, including the cloak of invisibility [1-11]. Over the last decade, hyperbolic metamaterials (HMMs) have gained a central role. HMMs are uniaxial structures that combine the properties of transparent dielectrics and reflective metals. The effective permittivity tensor has principal components of different signs. It can arise from excitation of coupled surface plasmons inside of HMMs. Surface plasmons arise in the metal flat surface adjacent to dielectric while localized surface plasmons arise if the metal has a shape of a nanoparticle or a nanowire. The excitation of plasmons is accompanied by the generation of electromagnetic field. If sub-wavelength metallic and dielectric layers create the periodic structure or metallic nanowires are periodically arranged in dielectric matrix with sub-wavelength separation, electromagnetic field of the separate plasmonic interfaces giving rise to a collective response. This collective response can be interpreted as originating from bulk effective media, possessing unique anisotropic dispersion relation, named hyperbolic. The interaction of HMMs with the near-field of a light source results in different applications starting from sub-wavelength light manipulation to many other pronounced physical effects [12-21]. Although the successful development of metamaterials has already been demonstrated, the next step in this very fast developing area of the modern physics and technique is required, namely, to find the way to make metamaterials tunable and adaptive. Tunable and adaptive materials can dynamically optimize themselves to fit their current operating environment. The tuning ability helps make metamaterial devices more versatile, adapting to shifting input or changing target parameters.

Project is directed on research of new structures containing metamaterials, which interact with incident electromagnetic waves and possess an optical tunability. In particular, such structures can be created by metallic nano-wires on glass substrate covered with isotropic/anisotropic matrix (liquid crystal/liquid crystal polymer) or represent the layered structures of the 2D conducting materials separated by dielectric layers. It also can be metasurface covered by liquid crystal or structure of type "grating-monolayer MoS_2-liquid crystal".

1. In the project we propose to utilize liquid crystals, as one possible way of solving the challenging problem of optical tunability of structures containing metamaterials. The main feature of liquid crystalline materials is their huge sensitivity to the external fields and thus ability to change physical properties considerably under small external fields. These enable the use of electric, magnetic or optical fields to control and tune the properties of the metamaterial.
2. We study the HMMs represented by the metallic nano-wires in the dielectric host matrix. As the host we use isotropic or anisotropic medium, e.g. liquid crystal. We also study a possibility to control surface plasmons in core-shell type nano-wires made of different materials and sandwich-type systems (film of Au/Ag with liquid crystal layer above it). Core-shell structure of the nano-wires gives additional possibility of tuning the HMMs. Shell may be radially anisotropic and inhomogeneous. We develop a theoretical approach and calculate the effective dielectric function of tunable isotropic/anisotropic host filled with the core-shell metallic nano-wires. In structures based on the graphene/MoS_2 layer the surface plasmon waves are excited using nano-gratings. We incorporate in these structures the liquid crystal layer, which provides the tuning of the light transmittance, absorption, and reflectance by reorienting the liquid crystal director. Metasurfaces have an advantage compared to the 3D metamaterials of occupying less physical space. We add a tunable liquid crystalline layer on top of the nonlinear metasurface (MoS_2) to control optical properties of the metasurface.

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Technical Approach

Dielectric Function of Metals.

Frequency of the plasmonic resonance in metallic layer depends on the dielectric function of the metal. Accounting for inter-band and intra-band transitions results in

$$\epsilon(\omega) = \epsilon_b(\omega) - \epsilon_\infty \frac{\omega_p^2}{\omega^2 + i\gamma_0\omega}$$

where the first term represents contribution from inter-band transitions that coexist with free-electron contribution presented by the second term in the Drude model; ω_p is plasma frequency.

Dielectric function of silver [1]

$$\epsilon_{\mathrm{Ag}}(\lambda) = \epsilon_\infty \left(1 - \frac{1}{\lambda_p^2\left(\frac{1}{\lambda^2} + \frac{i}{\mu_p\lambda}\right)}\right),$$
$$\text{where} \quad \epsilon_\infty = 4, \quad \lambda_p = 282\,\mathrm{nm}, \quad \mu_p = 17\,000\,\mathrm{nm},$$

Dielectric function of gold [2]

$$\boxed{\begin{aligned}
\epsilon_{\mathrm{Au}}(\lambda) \;&=\; \epsilon_\infty \left(1 - \frac{1}{\lambda_p^2\left(\frac{1}{\lambda^2} + \frac{i}{\mu_p\lambda}\right)}\right) \\
&\quad + \sum_{n=1,2} \frac{A_n}{\lambda_n}\left[\frac{e^{i\phi_n}}{\frac{1}{\lambda_n} - \frac{1}{\lambda} - \frac{i}{\mu_n}} + \frac{e^{-i\phi_n}}{\frac{1}{\lambda_n} + \frac{1}{\lambda} + \frac{i}{\mu_n}}\right], \\
\text{where} \quad &\epsilon_\infty = 1.54, \quad \lambda_p = 177.5\,\mathrm{nm}, \quad \mu_p = 14\,500\,\mathrm{nm}, \\
&A_1 = 1.27, \quad \phi_1 = -\pi/4, \quad \lambda_1 = 470\,\mathrm{nm}, \quad \mu_1 = 1900\,\mathrm{nm}, \\
&A_2 = 1.10, \quad \phi_2 = -\pi/4, \quad \lambda_2 = 325\,\mathrm{nm}, \quad \mu_2 = 1060\,\mathrm{nm}.
\end{aligned}}$$

Dielectric Function of Small Metallic Particles.

Permittivity of metal nanoparticles (NP) differs from bulk permittivity of medium. Finite size of metal particle leads to change in relaxation of electrons in conduction band. For instance permittivity of silver NPs can be estimated by classical model with constraint imposed on electron mean free path:

$$\varepsilon(\omega, r) = \varepsilon_b(\omega) + \frac{\omega_p^2}{\omega(\omega + i\gamma_0)} - \frac{\omega_p^2}{\omega(\omega + i\gamma)}, \qquad \gamma = \gamma_0 + v_F/r$$

ω is frequency of incident field, ω_p is plasma frequency, ε_b is experimentally determined permittivity for bulk sample, v_F is mean electron velocity at Fermi surface. For silver, $v_F = 1.39\times10^6$ m/s, $\gamma_0 = 0.018$ eV, $\omega_p = 9.02$ eV, γ_0 is electron relaxation rate in the metal, 2r is characteristic diameter of particle in field direction. For gold NP: $v_F = 1.4\times10^6$ m/s, $\gamma_0 = 0.027$ eV, $\omega_p = 9.04$ eV [3,4].

Classical Approach for Size-Dependence of Dielectric Function.

If particle size is comparable to or smaller than mean-free path of free conduction electrons in bulk material, ℓ_∞ (42 nm for Au, 52 nm for Ag and 45 nm for Cu), scattering of conduction electrons from particle surface results in a reduced effective mean-free path, $L_{eff} < \ell_\infty$ (free-path effect). Models for electron free have $\gamma = \gamma_0 + v_F / L_{eff}$. The quantum mechanical method based on Kramers–Heisenberg dispersion relation is used to evaluate the dielectric response of small metal particles (sphere, cylinder, rectangular prism, spherical shell, and cylindrical shell) [5]

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Dielectric Function of Non-Spherical Metallic Particles
Size effects are significant as dimensions become comparable to electron mean free path (50 nm for silver). Dielectric function may become anisotropic for nanostrips if size effect is significant.

Dielectric function of silver nanostrip of about 100nm size:

$$\varepsilon_m(\omega,\alpha,\beta) = 1 - \frac{\omega_p^2}{\omega(\omega - i\alpha\gamma_\infty)} + \frac{f\omega_L^2}{\omega_L^2 - \omega^2 + i\beta\Gamma_L\omega},$$

where $\omega_p = 9.17\,\mathrm{eV}$, $\gamma_\infty = 0.021\,\mathrm{eV}$, $f = 2.2$, $\omega_L = 5.27\,\mathrm{eV}$, $\Gamma_L = 1.14\,\mathrm{eV}$

α,β are fitting parameters. $\alpha=1,\beta=1$ for bulk silver [6].

Electron Free Path in Non-Spherical Particles.

$$\epsilon(\omega, L_{\text{eff}}) = \epsilon_{\text{bulk}}(\omega) + \frac{\omega_p^2}{\omega^2 + i\omega\gamma_0} - \frac{\omega_p^2}{\omega^2 + i\omega\left(\gamma_0 + A\dfrac{v_F}{L_{\text{eff}}}\right)}$$

Oblate spheroid

$$L_{\text{eff}} = \frac{2d}{\frac{3}{2} + \frac{3}{4}F_1} \qquad F_1 = \frac{(1-e^2)}{e}\ln\left(\frac{1+e}{1-e}\right)$$

where $e^2 = (1-r^2)$.

Prolate spheroid

$$L_{\text{eff}} = \frac{2d}{\frac{3}{2} + \frac{3}{2}F_2}, \qquad F_2 = \frac{\sin^{-1} e}{e}$$

Prism and cylinder (depending on the ration between particle dimensions, d is the height and D is one of the sides of the base

$$L_{\text{eff}} = \frac{2d}{2r+1} \qquad L_{\text{eff}} = \frac{2d}{r+2} \qquad r = d/D$$

Spherical Core-Shell Particle. Isotropic Shell.
Absorption by spherical nano-particle with core-shell structure is given approximately by

$$\sigma \approx \frac{2\pi}{\lambda}\mathrm{Im}[\alpha],$$

where polarizability of sphere covered with isotropic spherical layer is [7]:

$$\alpha = 4\pi R^3 \frac{(\varepsilon_S - \varepsilon_m)(\varepsilon_{Au} + 2\varepsilon_S) + f(\varepsilon_{Au} - \varepsilon_S)(\varepsilon_m + 2\varepsilon_S)}{(\varepsilon_S + 2\varepsilon_m)(\varepsilon_{Au} + 2\varepsilon_S) + 2f(\varepsilon_{Au} - \varepsilon_S)(\varepsilon_S - \varepsilon_m)}$$

where f is volume fraction of core, R is a radius of nano-particle, ε_{Au}, ε_S, ε_m are dielectric functions of nano-particle core, nano-particle shell and medium, respectively.

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Spherical Core-Shell Particle. Anisotropic Shell.

In paper [8] studying the Mie scattering by spherical particle with radial anisotropic shell the following result for leading scattering coefficient a_1 was obtained:

$$a_1 = -\frac{2}{3} i \left(\frac{2\pi (R+d)}{\lambda} \right)^3 \frac{\left[(S+1)\varepsilon_\parallel + \varepsilon_1 \right]\left[S\varepsilon_\parallel - \varepsilon_m \right] - f^{(2S+1)/3} \left[(S+1)\varepsilon_\parallel + \varepsilon_m \right]\left[S\varepsilon_\parallel - \varepsilon_1 \right]}{\left[(S+1)\varepsilon_\parallel + \varepsilon_1 \right]\left[S\varepsilon_\parallel + 2\varepsilon_m \right] - f^{(2S+1)/3} \left[(S+1)\varepsilon_\parallel - 2\varepsilon_m \right]\left[S\varepsilon_\parallel - \varepsilon_1 \right]}$$

$$(R+d)/R = f^{-1/3} \qquad S = \left(2\frac{\varepsilon_\perp}{\varepsilon_\parallel} + \frac{1}{4} \right)^{1/2} - \frac{1}{2}$$

where d is a thickness of shell, ε_1 is dielectric function of nano-particle core $\varepsilon_\parallel$, $\varepsilon_\perp$ are main values of anisotropic shell dielectric tensor.

Effective dielectric function of ensemble of core-shell Au nanoparticles [9]:

$$\varepsilon_{eff} = \varepsilon_h \left(1 + 3\eta \left(\frac{\varepsilon_{Au} - \varepsilon_h}{\varepsilon_{Au} + 2\varepsilon_h} \right) / \left(1 - \eta \frac{\varepsilon_{Au} - \varepsilon_h}{\varepsilon_{Au} + 2\varepsilon_h} \right) \right),$$

where ε_h is a dielectric function of host medium, η is a volume fraction of Au nanoparticles.

Excitation of Surface Plasmon.

We consider a nanorod-mediated surface plasmon resonance sensor and investigate the influence of its different structural parameters on the sensitivity enhancement. For this purpose we study a five-layer system depicted on Fig 1. The system includes the following elements: a glass prism (layer 1), liquid crystal (layer 2), a thin metal film (layer 3), a layer of aligned nanorods array (layer 4), and a sensing layer, which can be air or the target analyte (layer 5).

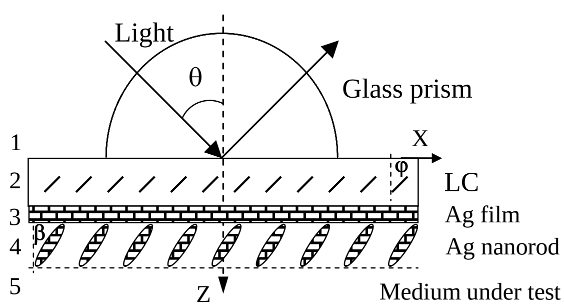

Fig.1. Schematic of a 5-layer glass prism-LC-metal film-nanorod array-sensing medium model. Voids between nanorods have the same material as the target analyte.

The theoretical modeling accounts for two anisotropic layers (liquid crystal layer and layer of metallic nanorods). It is based on five-layer Fresnel equations and the Maxwell-Garnett type effective medium theory [10, 11]. The effective medium theory is adopted to treat the nanorods and the voids between them as a layer with an effective dielectric constant. For simplicity it is assumed that the voids are made of the same material as the sensing layer.

We investigate the reflectance of the system in the environment with the refractive indices of 1.00 and 1.33 as a function of the light beam incidence angle. The nanorod-mediated surface plasmon resonance is studied depending on the nanorod tilt angle, concentration, length and diameter of nanorods, orientational state and thickness of the liquid crystal film.

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Method of Generating Function in Theory of Space-Time Transformation Media.

Let we have space (vacuum or air) which contains cloaking spherical shell with outer radius R_2 and inner radius R_1. Let us introduce the transformation of spherical coordinates as [12]

$$r^{'} = \frac{R_2}{R_2 - R_1}(r - R_1), \quad \theta^{'} = \theta, \quad \varphi^{'} = \varphi\,, \tag{1}$$

which connects spherical coordinates of point in the first space, $\{r^{'}, \theta^{'}, \varphi^{'}\}$, with coordinates of point in the second space, $\{r, \theta, \varphi\}$. The coordinate transformation (1) transforms the sphere of radius R_2 in the first space (we call it as the free space) into the spherical shell $R_1 < r < R_2$ in the second space (we call it as the real space). In Fig.1 we show for illustration the path of ray in the free(empty) space (a) and the path of the same ray in the real space defined by the coordinate transformation (1). Here a position of the spherical shell is also shown.(b).

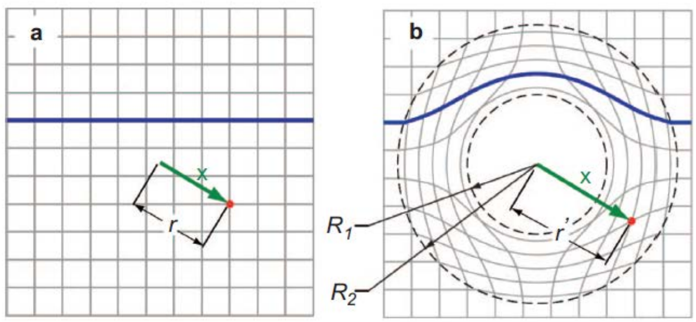

Fig.2. The path of the same ray and position of vector $\vec{x}$ in the free space (a) and in the space obtained under transformation (1) – (b). Position of the spherical shell in the space (b) is also shown [12].

The Maxwell equations in the free space

$$\nabla \times \vec{E}^{'} = -\mu_0 \frac{\partial \vec{H}^{'}}{\partial t}, \quad \nabla \times \vec{H}^{'} = -\varepsilon_0 \frac{\partial \vec{E}^{'}}{\partial t} \tag{2}$$

maintain their form under transformations (1) because of their form-invariant property and become

$$\nabla \times \vec{E} = -\hat{\mu} \frac{\partial \vec{H}}{\partial t}, \quad \nabla \times \vec{H} = -\hat{\varepsilon} \frac{\partial \vec{E}}{\partial t} \quad , \tag{3}$$

where $\vec{E}$ and $\vec{H}$ are the fields in the new coordinates, $\hat{\varepsilon}$ and $\hat{\mu}$ are tensors with the following components:

$$\frac{\varepsilon_r}{\varepsilon_0} = \frac{\mu_r}{\mu_0} = \frac{R_2}{R_2 - R_1}\frac{(r - R_1)^2}{r^2}, \frac{\varepsilon_\theta}{\varepsilon_0} = \frac{\mu_\theta}{\mu_0} = \frac{R_2}{R_2 - R_1}, \frac{\varepsilon_\varphi}{\varepsilon_0} = \frac{\mu_\varphi}{\mu_0} = \frac{R_2}{R_2 - R_1} \tag{4}$$

It means that if the permittivity and permeability components of the spherical shell satisfy the expressions (4), all of the light rays incident on the shell will be guided around the inner sphere with radius R_1 (see Fig. 2b). Therefore, the spherical shell with any object placed inside the shell will become invisible to outside observers.

It can be shown that in the case of the coordinate transformation of the type $r^{'} = r^{'}(r), \theta^{'} = \theta, \varphi^{'} = \varphi$ the next set of the expressions can be derived:

$$\frac{dr}{dr^{'}} = \frac{1}{\varepsilon_t(r)}, \quad \frac{r}{r^{'}} = \frac{1}{\sqrt{\varepsilon_t(r)\varepsilon_r(r)}}\,, \tag{5}$$

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where $\varepsilon_t(r)$ and $\varepsilon_r(r)$ are the relative tangential and radial, $0 < r' < R_2$, $R_1 < r < R_2$. Using (5) we can arrive at a differential equation as follows

$$\frac{d\left(r\sqrt{\varepsilon_t(r)\varepsilon_r(r)}\right)}{dr} = \varepsilon_t(r) \tag{6}$$

Equation (6) does not depend on the coordinate transformation and directly displays the expression that the permittivities of a spherical shell have to satisfy. We note that this approach is an inverse approach. The direct method is to find the permittivities from a known function of the coordinate transformation. The inverse approach derives the coordinate transformation from the known tangential and radial permittivities.

Integrating (6) and after some algebra we arrive at

$$\varepsilon_t(r) = \frac{R_2 g(r)}{\int_{R_1}^{R_2} g(r)dr}, \quad \varepsilon_r(r) = \frac{R_2\left(\int_{R_1}^{r} g(r)dr\right)^2}{r^2 g(r)\int_{R_1}^{R_2} g(r)dr} \tag{7}$$

The dimensionless generating function $g(r)$ is an arbitrary one. The limitations for $g(r)$ are connected only with conditions of the experimental realization of a cloak, in particular, with non-finite values of the permittivities.

<u>Cloaking Using Radial Anisotropy.</u> <u>Spherical Shell With</u> <u>Radially Inhomogeneous Permittivity.</u>

Laplace equation

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\,\varepsilon_r\frac{\partial\phi}{\partial r}\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\varepsilon_t\frac{1}{r}\frac{\partial\phi}{\partial\theta}\right) = 0\,, \tag{8}$$

where ϕ is the potential function, $\varepsilon_r = \varepsilon_{r0}r^m$, $\varepsilon_t = \varepsilon_{t0}r^m$ for $b \le r \le a$, $\varepsilon_r = \varepsilon_t = \varepsilon_i$ for $r \le b$, $\varepsilon_r = \varepsilon_t = \varepsilon_m$ for $r \ge a$. a is an outer radius of spherical shell, b is a radius of inclusion, ε_i and ε_m are permittivities of inclusion and external media, respectively.

Solution to eq.(8)

$$\begin{aligned}
\phi(r,\theta) &= Ar\cos\theta, \quad r \le b \\
\phi(r,\theta) &= \left(Br^{t_1} + Cr^{t_2}\right)\cos\theta, \quad b \le r \le a \\
\phi(r,\theta) &= \left(Fr^{-2} - E_0 r\right)\cos\theta \quad r \ge a
\end{aligned} \tag{9}$$

where

$$t_{1,2} = \frac{-(m+1) \pm \sqrt{(m+1)^2 + 8\dfrac{\varepsilon_{t0}}{\varepsilon_{r0}}}}{2} \tag{10}$$

Using boundary conditions we can find constants A, B, C, F in eq. (9).

Sphere is polarized by external electric field and creates electric potential $\phi = \alpha_s \frac{a^3}{3}\frac{\cos\theta}{r^2}E_0$ where α_s is a polarizability of the sphere. Comparing it with eq. (9) for $r \ge a$ we get expression for α_s. Then taking into account the Clausius-Mossotti formula, $\alpha_s = 3\frac{\varepsilon_{ef} - \varepsilon_m}{\varepsilon_{ef} + 2\varepsilon_m}$, we obtain the following expression for the effective permittivity of the sphere with inclusion:

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$$\varepsilon_{ef} = \varepsilon_m + \Delta\varepsilon_{ef}\,,\ \Delta\varepsilon_{ef} = \frac{\dfrac{2\xi}{(m+1)-\xi}[1-\dfrac{\varepsilon_m}{\varepsilon_i}(\dfrac{b}{a})^m]\left(\dfrac{b}{a}\right)^{\xi}}{[1-\dfrac{\varepsilon_m}{\varepsilon_i}(\dfrac{b}{a})^m]\left(\dfrac{b}{a}\right)^{\xi} - [1-\dfrac{(m+1)+\xi}{(m+1)-\xi}\dfrac{\varepsilon_m}{\varepsilon_i}(\dfrac{b}{a})^m]}, \qquad (11)$$

where $\xi = \sqrt{(m+1)^2 + 8\dfrac{\varepsilon_{t0}}{\varepsilon_{r0}}}$. In the ideal case the structure will be invisible if $\varepsilon_{ef} = \varepsilon_m$. But in real conditions to have more perfect invisibility we must minimize the value $\Delta\varepsilon_{ef}$.

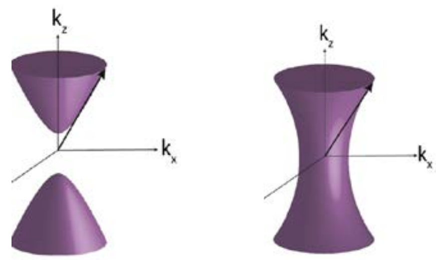
Hyperbolic Metamaterials (HMMs).

As is well-known, frequency ω and wave vector $\boldsymbol{k} = (k_x, k_y, k_z)$ of the extraordinary electromagnetic wave propagating in uniaxial anisotropic media satisfy to the dispersion relation

$$\frac{k_x^2 + k_y^2}{\varepsilon_{zz}} + \frac{k_z^2}{\varepsilon_{xx}} = \frac{\omega^2}{c^2}, \qquad (12)$$

where the permittivity components $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_\perp$, $\varepsilon_{zz} = \varepsilon_\parallel$.

When $\varepsilon_\parallel > 0, \varepsilon_\perp > 0$ the frequency surface (12) is an ellipsoid. However, when we have anisotropic media with $\varepsilon_\parallel \cdot \varepsilon_\perp < 0$, the isofrequency surface (12) opens into hyperboloid [Fig. 3(a, b)]. HMMs derive their name from this topology of the isofrequency surface. To create HMMs we need the material to behave like a metal in one direction and a dielectric in the other.



(a) (b)

Fig. 3. Hyperboloid isofrequency surface [13]. (a) $\varepsilon_{xx} = \varepsilon_{yy} > 0, \varepsilon_{zz} < 0$*; (b)* $\varepsilon_{xx} = \varepsilon_{yy} < 0, \varepsilon_{zz} > 0$.

Unique properties of HMMs are based on the excitation inside of HMMs of coupled surface plasmons (SP). A SP is an oscillation of electron density arising in a metal near its surface contacting with a dielectric. The excitation of electronic oscillations is accompanied by the generation of electromagnetic field. This field decays very fast with distance from surface on both the dielectric and metallic side creating the so-called near-field of the interface. The near-field is defined by distances shorter than the wavelength. Then, when the sub-wavelength metallic/dielectric layers are periodically stacked, or metallic nanowires are periodically arranged with the sub-wavelength separation in a dielectric matrix, the electromagnetic fields of the individual plasmonic interfaces overlap and couple, giving rise to a collective response. Such response can be interpreted as originating from bulk effective media with hyperbolic dispersion.

Currently, two structures are used for generation of hyperbolic dispersion relation: a stack of sub-wavelength alternating metallic and dielectric layers, and a lattice of metallic nanowires embedded in a dielectric matrix, termed nanowire array [Fig. 4(a, b)]. The optical response of these media can be homogenized via an effective medium theory allowing obtaining a hyperbolic effective permittivity tensor.

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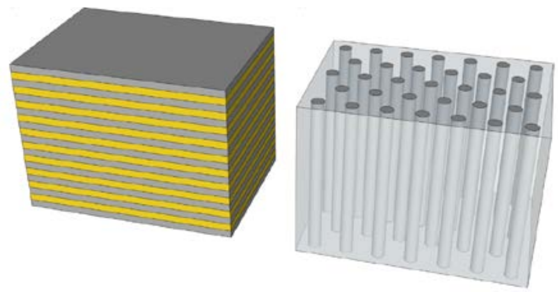

(a) *(b)*

Fig. 4. Schematics of a multilayer (a) and a nanowire (b) hyperbolic metamaterial [14].

<u>Cylindrical Core-Shell Nanowires Periodically Arranged in Dielectric Matrix</u>.

Each nanowire has a core-shell structure with a metallic core and a radially anisotropic dielectric shell. ε_c is the core permittivity, the main values of the shell permittivity tensor are denoted by $\varepsilon_\rho, \varepsilon_\varphi, \varepsilon_z$; a is an external radius of a shell, b is a radius of a core (Fig. 5).

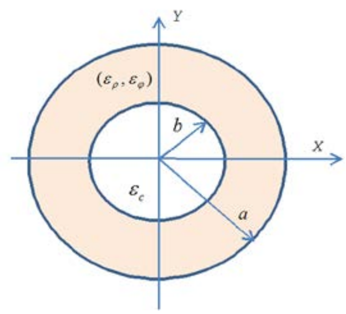

Fig. 5. Cross-section of a core-shell nanowire.

Effective permittivity tensor of a system of cylindrical core-shell nanowires periodically arranged in an isotropic dielectric matrix:

1) for the tensor component perpendicular to the nanowire ($\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_\perp$)

$$\varepsilon_\perp = \frac{(1+f)\varepsilon_m \varepsilon_{cyl,\perp} + (1-f)\varepsilon_m^2}{(1+f)\varepsilon_m + (1-f)\varepsilon_{cyl,\perp}}, \tag{13}$$

2) for the tensor component parallel to the z-axis (along the nanowire, $\varepsilon_{zz} = \varepsilon_\parallel$)

$$\varepsilon_\parallel = f\varepsilon_{cyl,\parallel} + (1-f)\varepsilon_m . \tag{14}$$

where ε_m is a permittivity of the dielectric matrix, f is the fill fraction of the nanowires, i.e. the ratio of the cross sectional area of a single nanowire to the cross sectional area of a metamaterial cell containing a nanowire, $\varepsilon_{cyl,\perp}$, $\varepsilon_{cyl,\parallel}$ are components of the cylindrical core-shell nanowire effective permittivity.

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In general case of the effective permittivity components of the core-shell nanowire with radially power-law dependent shell permittivity:

$$\varepsilon_{cyl,\perp} = \varepsilon_{\rho 0} \frac{t_2\left[t_1 \frac{\varepsilon_{\rho 0}}{\varepsilon_c}\left(\frac{b}{a}\right)^m - 1\right]\left(\frac{b}{a}\right)^{t_1-t_2} - t_1\left[t_2 \frac{\varepsilon_{\rho 0}}{\varepsilon_c}\left(\frac{b}{a}\right)^m - 1\right]}{\left[t_1 \frac{\varepsilon_{\rho 0}}{\varepsilon_c}\left(\frac{b}{a}\right)^m - 1\right]\left(\frac{b}{a}\right)^{t_1-t_2} - \left[t_2 \frac{\varepsilon_{\rho 0}}{\varepsilon_c}\left(\frac{b}{a}\right)^m - 1\right]} \tag{15}$$

$$\varepsilon_{cyl,\parallel} = \rho'\varepsilon_c + (1-\rho')\varepsilon_z\,, \tag{16}$$

where $\rho' = b^2/a^2$ is the metallic nanowire fill fraction.

Effective permittivity tensor of a system of cylindrical core-shell nanoparticles uniformly arranged in an anisotropic dielectric matrix (LC) [15]:

$$\varepsilon_\perp = \varepsilon_\perp^{LC} + f\frac{\left(\varepsilon_\perp^P - \varepsilon_\perp^{LC}\right)\varepsilon_\perp^{LC}}{\varepsilon_\perp^{LC} + (1-f)\,\tilde{\mu}_\perp\left(\varepsilon_\perp^P - \varepsilon_\perp^{LC}\right)}\,, \tag{17}$$

$$\varepsilon_\parallel = \varepsilon_\parallel^{LC} + f\frac{\left(\varepsilon_\parallel^P - \varepsilon_\parallel^{LC} + \nu\right)\varepsilon_\parallel^{LC} - \left(\varepsilon_\parallel^P - \varepsilon_\parallel^{LC}\right)\nu\tilde{\mu}_\parallel T_\parallel^0}{\varepsilon_\parallel^{LC} + (1-f)\,\tilde{\mu}_\parallel\left(\varepsilon_\parallel^P - \varepsilon_\parallel^{LC}\right) - f\nu\tilde{\mu}_\parallel T_\parallel^0}\,, \tag{18}$$

and

$$T_\parallel^0 = \frac{\varepsilon_\parallel^{LC}}{\varepsilon_\parallel^{LC} + \tilde{\mu}_\parallel\left(\varepsilon_\parallel^P - \varepsilon_\parallel^{LC}\right)} \tag{19}$$

Here $\varepsilon_\parallel^{LC}, \varepsilon_\perp^{LC}$, $\varepsilon_\parallel^P$, $\varepsilon_\perp^P$ are the LC and nanoparticle permittivity components along and perpendicular to the LC director, respectively, parameter ν describes the nanoparticle electric dipole, f is a volume concentration of nanoparticles. In particular, for prolate nanoparticles with long axis $c_n > a_n = b_n$ we can write

$$\tilde{\mu}_\parallel = \frac{1-e'^2}{e'^3}(\operatorname{arc\,tanh} e' - e'), \quad \tilde{\mu}_\perp = \frac{1}{2}(1-\tilde{\mu}_\parallel), \quad e' = \sqrt{1-\frac{\varepsilon_\parallel^{LC}}{\varepsilon_\perp^{LC}}\left(\frac{a_n}{c_n}\right)^2}\ . \tag{20}$$

In the case of cylindrical nanowires, $c_n \to \infty$ and we get $\tilde{\mu}_\parallel = 0, \tilde{\mu}_\perp = \frac{1}{2}$. At that we must replace the designations $\varepsilon_\parallel^P = \varepsilon_{cyl,\parallel}$, $\varepsilon_\perp^P = \varepsilon_{cyl,\perp}$, where $\varepsilon_{cyl,\perp}, \varepsilon_{cyl,\parallel}$ are defined by eqs.(15), (16).

The cylindrical core is metallic. For distinctness, we suppose that it is Au or Ag. In this case, the frequency dependence of permittivity is very well described by function presented in paper [16].

<u>Micro-Ribbon Grating Between the LC Slab and Isotropic Dielectric</u>.
We shall consider the Au/MoS_2 micro-ribbon grating placed between the LC slab and an isotropic dielectric. Under the incident light wave a surface plasmon (SP) is excited in the micro-ribbons. When excited on a periodical structure, a wave vector of the SP gets a phase shift due to the Bloch theorem and is adjusted to satisfy the momentum conservation law. Changing the grating spacing of the periodical structure we can obtain the SP excitation by the incident light wave from the desired range of wavelengths. We propose to control the absorption/reflection/transmission of the light wave reorienting the LC director of the LC slab.

To solve the problem we must find the LC director profile under applied electric field. The equilibrium director profile is found by minimizing the total free energy functional of the nematic LC sample. We take into account the following terms in the total free energy: the LC elastic energy term, coupling between the LC and nano-wires, interaction of the LC with electromagnetic field, the light field term.

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After minimization the LC free energy functional we obtain the Euler-Lagrange nonlinear equations for the LC director angles which are coupled with the Maxwell equations for electromagnetic waves in the LC. The Maxwell equations must be written and solved for electromagnetic fields in the LC, the nano-strips, and the isotropic dielectric substrate. Electromagnetic fields in these media are coupled via the boundary conditions. To calculate the dielectric permittivity of the nano-strips we use a model of Drude. The reflection and transmission coefficients are calculated using the formulae

$$R = \left|\mathrm{Re}(\mathbf{E}_r \times \mathbf{H}_r^*)\right| / \left|\mathrm{Re}(\mathbf{E}_i \times \mathbf{H}_i^*)\right|, \quad T = \left|\mathrm{Re}(\mathbf{E}_t \times \mathbf{H}_t^*)\right| / \left|\mathrm{Re}(\mathbf{E}_i \times \mathbf{H}_i^*)\right|. \tag{21}$$

The absorption coefficient is $A = 1 - (R + T)$. Here $\mathbf{E}_i, \mathbf{H}_i$, $\mathbf{E}_r, \mathbf{H}_r$, $\mathbf{E}_t, \mathbf{H}_t$ are electric and magnetic vectors of incident, reflected, and transmitted waves, respectively.

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Review of Technical Progress

Experimental design of plasmon systems often used in applications is studied. We considered and analyzed different models developed for calculation of dielectric function in metals, in particular, in gold and silver. Results of calculation in different models are compared with experimental data for dielectric function. In the case of gold and silver the models providing very good fit of the experimental data were selected.

Different models of metallic nano-particles and methods of describing their dielectric function were considered. We selected approaches and analytical expressions, which allow describing dielectric, function of nano-particles in the area of localized surface plasmon resonance. Using as an example of core-shell nano-particles the Au- core nanoparticle we studied and analyzed dependence of real and imaginary parts of dielectric function on wavelength in the cases of isotropic and anisotropic nano-particle shells.

Impact of nonlocality of dielectric function on optical response of metallic nanoparticles was considered. Methods of describing electro-magnetic wave interaction with single nanoparticles were also studied. We selected cases when exact solutions for electro-magnetic wave interaction with particles exist and are described by Mie-type theories. Special attention was spared to dielectric isotropic spherical particle and infinite cylindrical particle as examples of getting of Mie solution. In particular, we analyzed effect of finite size and particle shape on Fröhlich frequency. Among numerical methods used to study electro-magnetic wave interaction with nanoparticles we distinguished and considered Finite-Difference Time-Domain Method and Discrete Dipole Approximation.

Absorption in core-shell metal-dielectric nano-particles with isotropic and anisotropic shells and dielectric function of ensemble of spherical core-shell nanoparticles were studied. We have shown that core-shell metal-dielectric nano-particle provides opportunity to tune plasmonic resonance by changing properties of both core and shell. Adaptive core and/or shell may change their thickness (volume fraction) and dielectric constant under the action of external stimuli that finally results in shift of plasmonic frequency and change in absorption and scattering cross sections.

We considered a nanorod-mediated surface plasmon resonance sensor and investigated the influence of its different structural parameters on the sensitivity enhancement. The system includes the following elements: a glass prism, liquid crystal, a thin metal film, a layer of aligned nanorods array, and a sensing layer, which can be air or the target analyte. The theoretical modeling accounts for two anisotropic layers (liquid crystal layer and layer of metallic nanorods). It is based on five-layer Fresnel equations and the Maxwell-Garnett type effective medium theory. We investigated the reflectance of the system in the environment with the refractive indices of 1.00 and 1.33 as a function of the light beam incidence angle. The nanorod-mediated surface plasmon resonance is studied depending on the nanorod tilt angle, concentration, length and diameter of nanorods, orientational state and thickness of the liquid crystal film. It is shown that by controlling the orientational state of liquid crystal layer one can increase the sensitivity of the system.

Electric response of the objects covered by spherical and cylindrical shells under the quasi-static uniform electric field is studied. The permittivity of shells is radially anisotropic and its components depend on the distance to the shell center as r^m. We show that such shells can be used as invisibility cloak if radial and tangential components of the shell permittivity satisfy a certain relation between them. We considered media with permittivity not smaller than the vacuum permittivity and analyzed the efficiency of cloaking if: 1) external medium is vacuum, i.e. external medium permittivity $\varepsilon_m = 1$, 2) external medium permittivity $\varepsilon_m > 1$. In the first case only $m \geq 0$ are possible while in the second case the both $m \geq 0$ and $m < 0$ are possible. In the case $\varepsilon_m > 1$ we established conditions which allow reaching the ideal cloaking of inclusion by spherical or cylindrical shells at finite values of their permittivity components

It was shown that in the quasi-static limit the effective cloaking by spherical shell with radially dependent permittivity can be reached even if the shell permittivity is isotropic. We have analyzed dependence of the permittivity contrast parameter $\Delta\varepsilon_{ef}$ on the variation of the shell permittivity parameters for isotropic and anisotropic shells. It was established that variations of the shell radii ratio cause more strong impact on $\Delta\varepsilon_{ef}$ than variations of the shell permittivity parameters, $\varepsilon_{t0}, \varepsilon_{r0}, \varepsilon_{is,0}$. We have also shown that permittivity contrast parameter $\Delta\varepsilon_{ef}$ near the point of ideal invisibility has the same order for isotropic and anisotropic shells. The last observation can be considered as an argument in favor of more simple isotropic shells.

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We have studied the electrostatic responses of the cylindrical structures, which contain anisotropic cylindrical shell and magneto-optic core under steady homogeneous magnetic field. The permittivity components of cylindrical shell in the radial and tangential directions differ from each other and are radially inhomogeneous as r^m. We have shown that cylindrical shells with moderately large ratios of the radial and tangential permittivity components, $\varepsilon_{r0} / \varepsilon_{t0}$, can be used for cloaking magneto-optic inclusions in magnetic field. We have analyzed the efficiency of cloaking by cylindrical shells and have shown that more perfect invisibility of structures with magneto-optic core can be reached if the permittivity of the shells is radially inhomogeneous.

Theory of the space-time transformation and spatial transformation media is considered. Theory shows that transformation media that have holes in their coordinate grids in physical space can act as perfect invisibility devices: outside of the cloaking devices electromagnetic waves are indistinguishable from waves propagating through empty space. The device guides electromagnetic waves around the enclosed hidden object without causing disturbances. We considered and described the approach of the generating function to obtain the components of the radially anisotropic permittivity of the spherical shell providing the ideal invisibility of the cloaked object. This approach allows deriving the radial dependence of the permittivity components without knowing of the coordinate transformation. The coordinate transformation can now be derived from the known tangential and radial permittivities. We considered several types of the generating functions and calculated the radial dependence of the permittivity components created by these functions as well as the corresponding coordinate transformations. It gives a possibility to make easier a choosing the permittivity components radial dependence, which is more convenient for practical realization of the invisibility cloak.

We studied a system of cylindrical core-shell nanowires periodically arranged with the sub-wavelength separation in an isotropic dielectric matrix. Using theory of effective medium we carry out internal homogenization of radially anisotropic core-shell nanowires. Generalizing theory of homogenization of dielectric matrix with homogeneous inclusions for the case of matrix with inhomogeneous inclusions we used the core-shell nanowire effective permittivity tensor to obtain the effective permittivity tensor of the whole system. Basing on these results, we studied two cases: i) dielectric function of the nanowire shell is homogeneous, ii) dielectric function of the nanowire shell has radially power-law dependent components with exponent m.

In the case of homogeneous dielectric function of the nanowire shell it is shown that the system of the core-shell nanowires with the Au-core has properties of hyperbolic metamaterial (HMM) in the "low-frequency" area ($< (1-1.5)eV$) while the system of the core-shell nanowires with the Ag-core reveals the HMM properties in the both "low-frequency" ($< (1-1.5)eV$) and "high-frequency" ($> 3eV$) areas. The influence of parameters characterizing the system on the position and width of the HMM spectral regions is studied and conditions for broadening and shift of these regions are established.

If the dielectric function of the nanowire shell has radially power-law dependent components it is shown the following: 1) in the case of the nanowire Ag-core, the negative values of the exponent m provide tuning of the HMM area observed for homogeneous shell near the frequency 3.5 eV into the side of lower frequencies. Positive values of the exponent m lead to disappearance of this HMM area. Values of the exponent m practically do not influence the position of the HMM low frequency area below 2.0 eV; 2) in the case of the nanowire Au-core, the negative values of the exponent m lead to the appearance of the new frequency area (near 2 eV) where the system possesses the HMM properties.

It was established that replacing isotropic dielectric matrix by anisotropic one allows to widen the HMM frequency area near the frequency interval $\omega \approx (2.5-3.5)\,eV$ in the case of the Ag-core and obtain new HMM frequency area (near $\omega \approx 2\,eV$), which was absent in isotropic matrix in the case of the Au-core. We can tune the position and wide of the HMM frequency areas changing the parameters of nanowire or anisotropic dielectric matrix.

We studied a system of cylindrical core-shell nanowires periodically arranged with the sub-wavelength separation in the nematic liquid crystal (LC) matrix. The nanowire shell permittivity has radially power-law dependent components. We calculated components of the effective permittivity tensor of the system under consideration when the nanowire core is Ag and Au, and the LC matrix is the LC 5CB and LC E7. It is established that two frequency areas of the HMM properties can be obtained in the systems with the nanowire Ag-core and with the nanowire Au-core. Choosing values

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of the nanowire shell permittivity parameters we can change the position of the HMM areas. We studied influence of the LC matrix orientational states on the HMM area position, namely, the LC director is oriented parallel to the nanowires and the LC director is disordered (isotropic state). It is shown that one of the HMM areas in both systems, with the Ag-core and Au-core of the nanowires, is sensitive to the orientational state of the LC matrix. Thus, changing the orientational state of the LC matrix one can tune these HMM areas.

Light reflectance and transmittance of the three-layer system, isotropic dielectric – the paired gold nanowires grating – vanadium dioxide, was studied at the normal incidence of the light wave. Under the incident light wave the surface plasmon (SP) is excited in the gold nanowires that is observed in the spectral distribution of reflectance and transmittance of the system. Vanadium dioxide (VO_2) exhibits a transition from the semiconducting phase to the metallic phase at the temperature ~ 66 °C. At the phase transition the dielectric properties of VO_2 change significantly influencing the SP resonance frequency and transmittance/reflactance of the system. We observe the minimum in the transmittance/reflactance spectra of the system, which is identified with the SP excitation in the gold nanowires. Our modeling shows that we can effectively change transmittance/reflectance of the system on the SP resonance frequency by varying temperature from below to above the transition temperature semiconductor-metal in VO_2. We can also manage the SP resonance frequency in the visible or infrared ranges tuning parameters of the system. The suggested scheme may be used for modulators and filters in visible and infrared ranges.

Transmittance of the three-layer system, nematic LC – the paired gold nanowires grating – isotropic dielectric was studied for different values of the applied external voltage, which reorients the LC director. For calculation of the transmittance, we have developed codes in Matlab and Comsol Multiphysics software. We observe the minimum in the transmittance spectra of the system, which corresponds to the excitation of the SP polaritons in the gold nanowires. It is shown that the transmittance minimum position depends on the applied voltage. Therefore, we can tune the transmittance of the three-layer system changing the LC director orientational state.

Impact of the LC orientational state on the surface plasmon absorption spectra is studied in the case of the MoS_2 micro-ribbon grating placed between a nematic LC W1791 and an isotropic dielectric Si. The maxima in the absorption spectra corresponding to the excitation of the surface plasmons in the MoS_2 micro-ribbons, are observed in the (30-2.1) THz range. We show that the maxima magnitude depends on the LC orientational state. The influence of the LC director orientation increases with increasing the MoS_2 micro-ribbon width. The results suggest that control of the orientational state of the nematic LC layer enables us to manipulate the absorption maxima value. We also can manage the resonance frequency of the surface plasmons in the infrared range tuning parameters of the system.

The SP absorption spectrum was studied in the structure composed of the graphene-MoS_2 micro-ribbon grating placed between a nematic LC and an isotropic dielectric Si. The maxima in the absorption spectra, which are related to the excitation of the SP in the graphene and MoS_2 micro-ribbons were observed. The absorption peaks are splitted in comparison with those observed in the MoS_2 grating and shifted into the short wavelengths side. As in structure with the MoS_2 grating the magnitude of the absorption peaks can be controlled by the director orientation of the nematic LC layer.

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Summary of Individual Research Contributions

Professors of Taras Shevchenko National University of Kyiv, V. Reshetnyak and I. Pinkevych, Drs. O. Romanenko, S. Bielykh, and V. Zadorozhnii, and student E. Cheypesh fulfilled tasks of the project during the reported period.

Prof. V. Reshetnyak developed a theory of surface plasmons of nanoparticles in nematic liquid crystals;

- developed a theory of plasmons in core-shell type nanoparticles;
- developed a theory of plasmons in ensemble of core-shell type nanoparticles;
- developed a theory of the physical mechanisms responsible for tuning of index function in metamaterials with the liquid crystals;
- developed a theory of the physical mechanisms responsible for tuning of index function and calculated index function for spherical shells;
- calculated the effective dielectric function of metamaterials based on liquid crystals
- developed the transformational optics concept for anisotropic inhomogeneous tunable metamaterials based on liquid crystalline matrix and methods of solving the inverse problem;
- developed a theoretical approach and model of interaction of incident electromagnetic wave with metallic nano-wires on glass substrate;
- obtained equations describing the interaction of electromagnetic wave with nano-wires in isotropic host;
- obtained equations describing the interaction of electromagnetic wave with nanowires in aniisotropic host;
- obtained equations describing the interaction of electromagnetic wave with nanowires in the aniisotropic LC host;
- developed a theoretical approach describing the electromagnetic wave transmittance and reflectance from the layered structure containing "grating-graphene/monolayer MoS2 –liquid crystal";
- developed a theoretical approach describing the electromagnetic wave transmittance and reflectance from the layered structure containing "isotropic dielectric – the paired gold nanowires grating – vanadium dioxide";
- developed a theoretical approach describing the electromagnetic wave transmittance and reflectance from the layered structure containing "grating MoS2 – liquid crystal”;
- developed a theoretical approach describing the electromagnetic wave transmittance and reflectance from the layered structure containing "grating raphene-MoS2 – liquid crystal”.

Prof. I. Pinkevych developed a theory of dielectric function of metallic and ferroic nanoparticles;

- developed a theory of dielectric function of core-shell type nanoparticles;
- developed a theory of dielectric function of chain of spherical core-shell type nanoparticles;
- developed a theory of the physical mechanisms responsible for tuning of index function in metamaterials with the liquid crystal polymers;
- developed methods of calculation of the surface plasmon frequency in sandwich-type systems;
- developed a theory of the physical mechanisms responsible for tuning of index function with imaginary part and calculated index function for cylindrical shells;
- calculated the effective dielectric function of cylindrical shells with optic active metallic core in magnetic field;
- developed the transformational optics concept for anisotropic inhomogeneous tunable metamaterials based on elastomer and methods of solving the inverse problem;
- developed the transformational optics concept for anisotropic inhomogeneous tunable metamaterials based on elastomer and methods of solving the inverse problem;
- studied the influence of the nano-wire core-shell structure on interaction with electromagnetic wave;
- solved equations describing the interaction of electromagnetic wave with nano-wires in isotropic host;
- solved equations describing the interaction of electromagnetic wave with nanowires in aniisotropic host;
- solved equations describing the interaction of electromagnetic wave with nanowires in the aniisotropic LC host;
- calculated coefficients of the transmission and reflection from the layered structure of type "grating-graphene/monolayer MoS 2 -liquid crystal";
- calculated coefficients of the transmission and reflection from the layered structure "isotropic dielectric – the paired gold nanowires grating – vanadium dioxide";
- calculated coefficients of the transmission and reflection from the layered structure of type "grating MoS_2 -liquid crystal";
- calculated coefficient of absorption in the layered structure of type "grating graphene-MoS_2 -liquid crystal".

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Dr. V. Zadorozhnii developed methods of generalization of the Maxwell-Garnett theory for the case of liquid crystals and for metamaterials based on liquid crystals;

- developed methods of calculation of light reflection coefficient in metamaterials based on liquid crystals;
- calculated the surface plasmon frequency in sandwich-type system: film of Ag - LC layer filled with nano-particles;
- calculated the effective dielectric function of anisotropic systems;
- developed the methods of solving the inverse problem and deriving the appropriate effective dielectric/magnetic tensors.

Dr. S. Bielykh developed the Bruggeman theory for the case of liquid crystals and for metamaterials based on liquid crystals;

- calculated the effective dielectric function of metamaterials based on liquid crystals.

Dr. O. Romanenko studied and developed methods of calculating the effective electromagnetic parameters;

- studied and developed methods of calculating the effective electromagnetic parameters of metamaterials based on liquid crystals.

Student E. Cheypesh developed the code for numerical calculation of electromagnetic wave interaction with nanowire;

- provided numerical calculations of the equations and plotting.

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Publications

The following technical articles were published by researchers in this task.

1. V. Yu. Reshetnyak, I. P. Pinkevych, A. M. Urbas, D. R. Evans. Controlling hyperbolic metamaterials with a core-shell nanowire array [Invited], Optical Materials Express, 2017, v.7, N2, pp. 542-554.
2. V. Yu. Reshetnyak, I. P. Pinkevych, T. J. Sluckin, and D. R. Evans. Cloaking by shells with radially inhomogeneous anisotropic permittivity, Opt. Express, 2016, v. 24(2), pp. A21-A32.
3. V. Yu. Reshetnyak, I. P. Pinkevych, V. I. Zadorozhnii and D. R. Evans. Liquid Crystal Control of Surface Plasmon Resonance Sensor Based on Nanorods, Mol. Cryst. Liq. Cryst., 2015, v.613, pp.110-120.
4. V. Reshetnyak, I. Pinkevych, A. M. Urbas, and D. R. Evans, Managing Hyperbolic Metamaterial with Core-Shell Nanowire Array, 1-th International Conference on Optics, Photonics and Materials, 26-28 October 2016, Nice, France.
5. P. Pinkevych, V. Yu. Reshetnyak, D. R. Evans, Influence of cholesteric liquid crystal elastic properties on the two light beam energy exchange, Conference "Microscale Ocean Biophysics" co-organized with COST Action MP1305 "Flowing Matter", 31 October – 4 November 2016, Eilat, Israel.
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7. V.I. Zadorozhnii, V.Yu. Reshetnyak, I.P. Pinkevych, and D.R. Evans, Using liquid crystal layer to tune the surface plasmon resonance in a sensor based on substrate decorated with nanorods, Workshop "Complex Liquids at Structured Surfaces", 24-28 February 2015, Berlin, Germany.
8. Igor P. Pinkevych, Victor Yu. Reshetnyak, Tim J. Sluckin, Dean R. Evans, Impact of cholesteric liquid crystal structure in hybrid photorefractive cells on the two beam energy exchange, Workshop "Complex Liquids At Structured Surfaces", 24-28 February 2015, Berlin, Germany.
9. Victor Reshetnyak, Igor Pinkevych, Victor Zadorozhnii Dean R. Evans, Liquid crystal control of nanoparticles-mediated surface plasmon resonance sensor, 8th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics – Metamaterials 2014, 25-30 August 2014, Copenhagen, Denmark.
10. Igor Pinkevych, Victor Reshetnyak, Dean Evans. Cloaking by shells with radially inhomogeneous permittivity, 8th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics – Metamaterials 2014, 25-30 August 2014, Copenhagen, Denmark.
11. Victor Reshetnyak, Igor Pinkevych, Dean R. Evans, Effective dielectric function of liquid crystal doped with radially anisotropic core-shell nanoparticles, 25-th International Liquid Crystal Conference, June 29 – July 4 2014, Dublin, Ireland.
12. Igor P. Pinkevych, Victor Yu. Reshetnyak, Victor I. Zadorozhnii, Dean R. Evans, Liquid Crystal Control of Surface Plasmon Resonance Sensor Based on Nanorods, 25-th International Liquid Crystal Conference, June 29 – July 4 2014, Dublin, Ireland.
13. Victor Reshetnyak, Igor Pinkevych, Tim Sluckin, Dean R. Evans, Novel Metamaterials based on Liquid Crystal filled with Core-Shell Nanoparticles, 12th International Photorefractive Review, 9-14 June 2014, Key Largo, Florida, USA
14. Igor P. Pinkevych, Victor Yu. Reshetnyak, Victor I. Zadorozhnii, Dean R. Evans. Liquid crystal control of surface plasmon resonance sensor based on nanorods, Physics of Liquid Matter: Modern problems(PLMMP-2014), 23-27 May 2014, Kyiv, Ukraine.
15. Victor Yu. Reshetnyak, Igor P. Pinkevych, Victor I. Zadorozhnii, Dean R. Evans, Liquid crystal control of surface plasmon resonance sensor based on nanorods. Cost Action MP0902, Topical Meeting on Nanoparticle-polymer composites, 14-15 October 2013, Heraklion, Crete, Greece.
16. Igor P. Pinkevych, Victor Yu. Reshetnyak, Tim Sluckin, Gary Cook, Dean R. Evans, Dynamic director grating and two beam energy exchange in photorefractive hybrid cholesteric cell. 7th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics, "Metamaterials 2013", 16-21 September 2013, Bordeaux, France.
17. Victor Yu. Reshetnyak, Igor P. Pinkevych, Augustine Urbas, Dean R. Evans, Plasmonic Resonance in Polymer Matrix Filled with Core-Shell Nanoparticles. Cost Action MP0902, Meeting on Composites of inorganic nanotubes and polymers, 20-22 March 2013, Ercolano, Italy.
18. Victor Yu. Reshetnyak1, Igor P. Pinkevych, Augustine Urbas, Dean R. Evans, Plasmonic Resonance in Liquid Crystal Filled with Golden Core-Shell Nanoparticles, 15-th Topical Meeting on Optics of Liquid Crystals, September 29 - October 4, 2013, Honolulu, Hawaii, USA.

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19. Igor P. Pinkevych, Victor Yu. Reshetnyak, Renato Torre, Theoretical modeling of transient grating in inorganic–elastomer nanocomposites. 6th COINAPO Topical Meeting, 19-21 November 2012, Rehovot, Israel.
20. V.I. Zadorozhnii, K.V. Bashtova, V.Yu. Reshetnyak,. Magneto-optical effects in twisted nematic liquid crystals doped with ferromagnetic particles. 2nd Workshop on Complex Liquids at Structured Surfaces, 10-12 October 2012, Lisbon, Portugalia.

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