# Dispersion Characteristics of Zinc Oxide Nanorods Organaized in Two-dimensional Uniform Arrays

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**Abstract**— The electromagnetic waves propagation in a two-dimensional periodic array of zinc oxide nanowaveguides covered with a thin metal film is solved by the separation of variables method in cylindrical coordinates. The numerical results obtained by our method are in good agreement with the ones computed by the commercial software COMSOL Multiphysics™ over all optical range and have minor deviations for the wavelength range close to the critical wavelength. Resonances located at the amplitude-frequency characteristics of optical nanoantennas may be interpreted as resonances of circular bilayer nanowaveguide segments with the ZnO core covered with thin metal shell. The results may also be used to predict the resonant wavelength of two-dimensional periodic arrays of ZnO nanorods coated with a thin metal layer and grown on a dielectric substrate.

## 1. INTRODUCTION

The new design of optical antennas based on the ZnO nanorods coated with a thin metal film is discussed in the paper [1]. The diffraction of electromagnetic waves by a single metal-dielectric nanooscillator and array of ones placed at the interface between dielectric layers has been solved. The dependencies of electrodynamic characteristics of optical antennas on the geometrical parameters were compared with the experimental data. Resonances located at the amplitude-frequency characteristics of optical nanoantennas may be interpreted as resonances of circular bilayer nanowave guide segments with the ZnO core covered with thin metal shell. In this regard it is of interest to investigate the range of the optical characteristics of similar waveguides.

The calculated dispersion characteristics of single waveguide and two-dimensional periodic arrays of ones are discussed in this paper. The dielectric constant dispersion of ZnO [2] and metal [3] were took into account. The metals are known to have a finite complex dielectric constant in the optical range.

## 2. STATEMENT OF THE PROBLEM

The Fig. 1 shows the geometry of optical waveguide composed of a core covered by a thin metal shell. The core has a radius $R_1$ and a dielectric constant $\varepsilon_1$. The shell with a dielectric constant $\varepsilon_2$ has a radius $R_2$. The thickness of the shell is $d = R_2 - R_1$. We assume that the dielectric constant $\varepsilon_3$ outside of the waveguide is equal to free space permittivity. The magnetic permeability

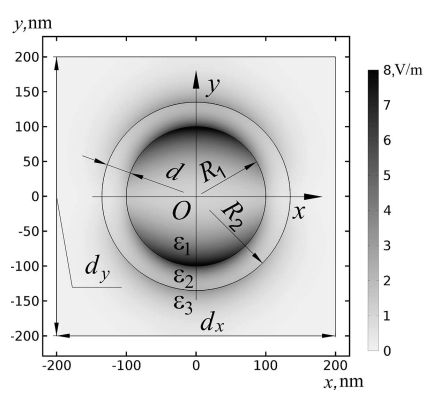


Figure 1: The electric field of the cylindrical nanowaveguide with $\lambda = 450\,\text{nm}$, $R_1 = 100\,\text{nm}$, $\varepsilon_1 = 4.0397 + 0.002i$ (ZnO), $R_2 = 135\,\text{nm}$, $\varepsilon_2 = 6.0830 + 0.7462i$ (Ag), $\varepsilon_3 = 1$, $d_x = d_y = 400\,\text{nm}$.

$\mu$ everywhere is equal to free-space permeability. The geometry shown in Fig. 1 of optical waveguide is described by Cartesian rectangular coordinate system. The $x$- and $y$-axis are the longitudinal coordinate. The $z$ axis is directed along the waveguide being unlimited in this direction. The parameters $d_x$ and $d_y$ are periods of the array along $x$ and $y$ axes, respectively.

The method of separation variables in cylindrical coordinate system ($r$, $\phi$, $z$) is applied to determine the frequency dependence of the complex propagation constant $\gamma(\omega)$ in the nanoantennas.

The electromagnetic field in the waveguide can be written by the longitudinal component of the electric $P^e(r,\phi)\exp(-i\gamma z)$ and magnetic $P^\mu(r,\phi)\exp(-i\gamma z)$ Hertz vector.

The solution of Helmholtz equation for waveguide arrays is assumed in the form:

$$P^e(r,\phi)=\sum_{m=1}^{\infty}\hat{P}_m^e(r)\sin m\phi,\quad P^\mu(r,\phi)=\sum_{m=1}^{\infty}\hat{P}_m^\mu(r)\cos m\phi \tag{1}$$

where $m$ is the azimuthal wave mode number. The summing symbol in (1) should be omitted in case of a single waveguide. The function $\hat{P}_m^{e,\mu}(r)$ may be written:

- in the core of the waveguide ($r \leq R_1$):

$$\hat{P}_m^{e,\mu}(r)=A_m^{e,\mu}\frac{\hat{J}_m(r)}{\eta_1^2\hat{J}_m(R_1)}, \tag{2}$$

- in the shell ($R_1 \leq r \leq R_2$):

$$\hat{P}_m^{e,\mu}(r)=\frac{1}{\eta_2^2\Phi_m^{(2)}(R_1,R_2)}\left[A_m^{e,\mu}\Phi_m^{(2)}(r,R_2)-C_m^{e,\mu}\Phi_m^{(2)}(r,R_1)\right], \tag{3}$$

- in free space ($r \geq R_2$) in case of a single waveguide:

$$\hat{P}_m^{e,\mu}(r)=C_m^{e,\mu}\frac{\hat{K}_m(r)}{\eta_3^2\hat{K}_m(R_2)}, \tag{4}$$

- in free space ($r \geq R_2$) in case of a periodic waveguide array:

$$\hat{P}_m^{e,\mu}(r)=\frac{1}{\eta_3^2\Phi_m^{(2)}(R_2,R_3)}\left[C_m^{e,\mu}\Phi_m^{(2)}(r,R_3)-B_m^{e,\mu}\Phi_m^{(3)}(r,R_2)\right], \tag{5}$$

where $R_3$ is an arbitrary radius, satisfying the condition $R_3>\sqrt{d_x^2+d_y^2}/2$. In Eqs. (2)–(5) we use

$$\hat{J}_m(r)=\begin{cases}\mathrm{J}_m(\eta_1 r), & \eta_1^2\geq 0,\\ \mathrm{I}_m(\eta_1 r), & \eta_1^2<0,\end{cases}\quad \hat{K}_m(r)=\begin{cases}\mathrm{N}_m(\eta_3 r), & \eta_3^2\geq 0,\\ \mathrm{K}_m(\eta_3 r), & \eta_3^2<0,\end{cases}$$

$$\Phi_m^{(j)}(r,d)=\begin{cases}\mathrm{J}_m(\eta_j r)\,\mathrm{N}_m(\eta_j d)-\mathrm{N}_m(\eta_j r)\,\mathrm{J}_m(\eta_j d), & \eta_j^2\geq 0,\\ \mathrm{I}_m(\eta_j r)\,\mathrm{K}_m(\eta_j d)-\mathrm{K}_m(\eta_j r)\,\mathrm{I}_m(\eta_j d), & \eta_j^2<0,\end{cases}$$

$A_m^{e,\mu}=\begin{Bmatrix}E_{z,m}(R_1)\\ H_{z,m}(R_1)\end{Bmatrix}$, $C_m^{e,\mu}=\begin{Bmatrix}E_{z,m}(R_2)\\ H_{z,m}(R_2)\end{Bmatrix}$, $B_m^{e,\mu}=\begin{Bmatrix}E_{z,m}(R_3)\\ H_{z,m}(R_3)\end{Bmatrix}$ are an unknown coefficients, $E_{z,m}$ and $H_{z,m}$ are longitudinal components of the electromagnetic field, $\eta_j^2=k^2\varepsilon_j-\gamma^2$, $k$ is a wavenumber, $J_m(z)$ is the Bessel function, $I_m(z)$ is the modified Bessel function, $N_m(z)$ is the Neumann function, $K_m(z)$ is the Macdonald function.

The solution is an ordinary in case of a single waveguide except the Hertz vector that can be written in form (2)–(5) satisfying the continuity condition of the longitudinal component of the electromagnetic field in boundaries $r=R_{1,2}$. The components $E_{\phi,m}(r)$, $H_{\phi,m}(r)$ should be found in each waveguide region considering boundary conditions. The solution may be written as system of linear algebraic equations (SLAE) for the four unknown coefficients. The dispersion relation is obtained by calculating the determinant of the SLAE being equated to zero.

In Eq. (5) we use an arbitrary radius $R_3$ and additional unknown coefficients $B_m^{e,\mu}$ in case of two-dimensional periodic array of zinc oxide nanowaveguides. The unknown coefficients $A_m^{e,\mu}$ and

$B_m^{e,\mu}$ may be omitted by using the continuity condition of azimuthal components $E_{\phi,m}(r)$, $H_{\phi,m}(r)$ on boundaries $r = R_{1,2}$. Lets sum in (1) for $m \leq M$, $M \gg 1$ values and require satisfaction the boundary conditions of $H_z(r,\phi) = 0$ in $M$ values on the side of the cell $x = d_x/2$ and $E_z(r,\phi) = 0$ in $M$ values on the top side of the cell $y = d_y/2$. These conditions are valid for waves in the array of waveguides excited by a normal incidence plane wave with polarization along the $y$-axis. The dispersion relation is also obtained by finding the determinant of the SLAE being equated to zero for unknown coefficients $C_m^{e,\mu}$.

The propagation constant in waveguides with complex permittivity has a complex value. It is very difficult to locate complex roots of a complex function at the complex plane. To solve this issue we use the Cauchy's argument principle [7].

Only waves with low losses has a wide range of practical applications. In this case we may simplify the finding complex roots method [8,9]. The propagation constant may be assumed as $\gamma(\varepsilon' - i\varepsilon'')$. Lets expand it in a Taylor and take three terms of the series:

$$\gamma\left(\varepsilon' - i\varepsilon''\right) \approx \gamma\left(\varepsilon'\right) - i\varepsilon''\gamma'\left(\varepsilon'\right) - \left(\varepsilon''\right)^2 \gamma''\left(\varepsilon'\right)/2.$$

The derivatives don't depend on the direction because the function $\gamma(\varepsilon)$ is an analytic. Therefore, we replace derivatives by finite differences:

$$\varepsilon''\gamma'\left(\varepsilon'\right) \approx \gamma\left(\varepsilon'\right) - \gamma\left(\varepsilon' - \varepsilon''\right), \quad \left(\varepsilon''\right)^2 \gamma''\left(\varepsilon'\right) \approx \gamma\left(\varepsilon' + \varepsilon''\right) + \gamma\left(\varepsilon' - \varepsilon''\right) - 2\gamma\left(\varepsilon'\right).$$

Hence

$$\gamma\left(\varepsilon' - i\varepsilon''\right) \approx \gamma\left(\varepsilon'\right) - i\left[\gamma\left(\varepsilon'\right) - \gamma\left(\varepsilon' - \varepsilon''\right)\right] - \left[\gamma\left(\varepsilon' + \varepsilon''\right) + \gamma\left(\varepsilon' - \varepsilon''\right) - 2\gamma\left(\varepsilon'\right)\right]. \tag{6}$$

Using this approach, the three real propagation constants of waveguide with a real permittivity should be found and applied the expression (6) to them to determine the complex propagation constant. The detailed analysis and verification of the numerical method described in this paper are shown in [8,9]. The calculation error increases sharply when $n''/n' > 0.1$ where $\gamma/k = n' - in''$. So, if we use the silver as a coating film, the fairly large errors are in the wavelength range 400–440 nm.

## 3. RESULTS AND DISCUSSIONS

The numerical results for $EH_{11}$ mode of the waveguide with radius $R_1 = 100$ nm covered by silver thin film having different thicknesses close to 40 nm are presented in this paper. These geometrical parameters are typical for ZnO nanorods [1,4,5].

The Fig. 2 shows the dispersion curves of the wave mode $EH_{11}$ of a single waveguide with the various shell thicknesses $d$. It also displays the refractive index ZnO $n_{\text{ZnO}}$ (curve 5). The

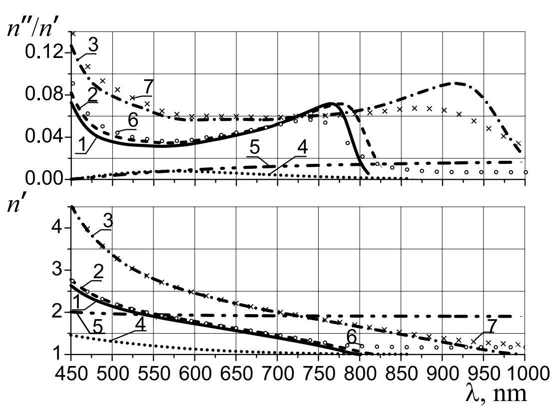


Figure 2: Dispersion curves of the optical waveguide with different shell thicknesses $d$: 1 — 45 nm, 2 — 35 nm, 3 — 15 nm, 4 — 0, 5 — ZnO, 6 — 35 nm (FEM), 7 — 15 nm (FEM).

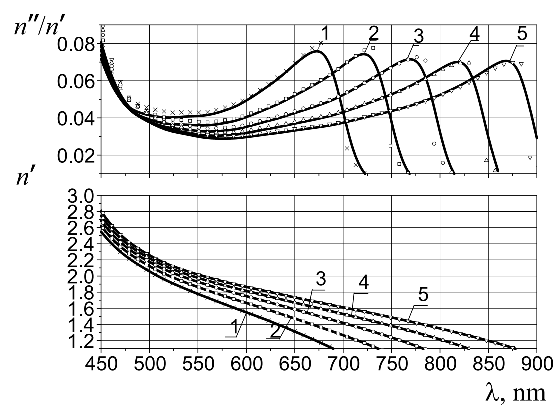


Figure 3: Dispersion curves of the waveguide with fixed shell thickness $d = 40$ nm and different core radiuses $R_1$: 1 — 80 nm, 2 — 90 nm, 3 — 100 nm, 4 — 110 nm, 5 — 120 nm. The results obtained by FEM in COMSOL Multiphysics$^{\text{TM}}$ are marked by symbols.

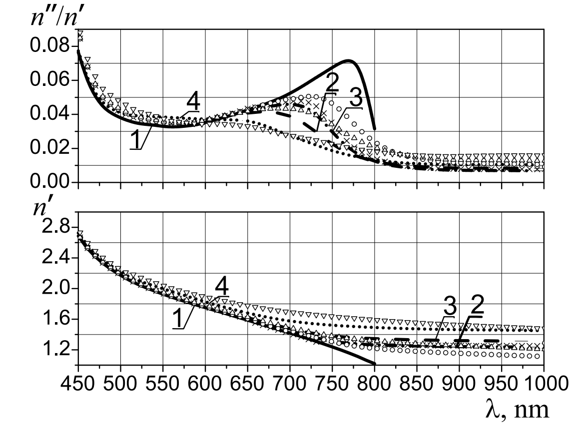


Figure 4: Dispersion curves of the array of waveguides with $R_1 = 100$ nm, $R_2 = 140$ nm and various unit cell size: 1 — single waveguide, 2 — array of waveguides with $d_x = d_y = 350$ nm, 3 — 325 nm, 4 — 300 nm. The results obtained by FEM are marked by symbols.

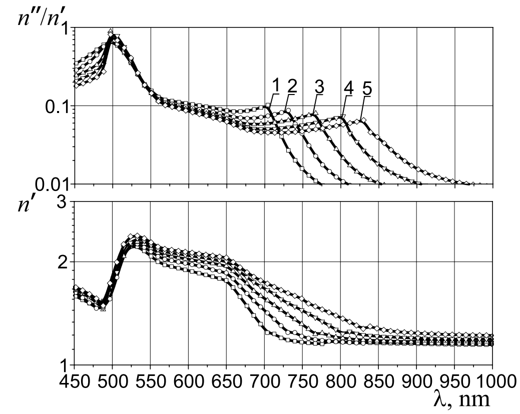


Figure 5: Dispersion curves of the mode $EH_{11}$ of the waveguide calculated by FEM with gold shell thickness $d = 40$ nm and different core radiuses $R_1$: 1 — 80 nm, 2 — 90 nm, 3 — 100 nm, 4 — 110 nm, 5 — 120 nm.

surface plasmon-polaritons ($E$-waves) localized near the boundary of ZnO-Ag can be excited in wavelength range where $n > n_{\mathrm{ZnO}}$. When the refractive index $n < n_{\mathrm{ZnO}}$, the volume wave localizes in the waveguide and decreases exponentially outside it. The waveguide properties don't depend on thickness of the silver shell $d$, when the thickness $d$ is greater than 30nm. The properties of the metal in optical waveband will close to microwave waveband when the wavelength increases. Therefore, the fundamental wave mode in the bilayered waveguide ZnO-Ag in contrast to a dielectric waveguide has a limited critical wavelength.

The dispersion curves in Fig. 2 with a shell thickness $d = 35$ nm (curve 6) and 15 nm (curve 7) are computed by COMSOL Multiphysics$^{\mathrm{TM}}$ platform of finite-element physics-based modeling and simulation. As the advantages of using the finite element method (FEM) for the numerical calculation of the optical layered structures properties [10], we may highlight the conservatism and high stability of the numerical method, the ability to solve problems with a complicated geometry and to reduce the mesh in those places where special care isn't required. Comparing the data of curves 2 and 3, 6 and 7, we can see that the results are in good agreement with the results of simulation in COMSOL Multiphysics$^{\mathrm{TM}}$. Dispersion characteristics are calculated by FEM have minor differences in the waveband close to the critical wavelength.

If we increase waveguide radius as shown in Fig. 3, the wave retardation coefficient will increases too and the losses will become considerably lower.

The wave mode $EH_{11}$ has a strong field localization in the waveguide in optical wavelength range, thus the dispersion properties of a periodic waveguide array as shown in Fig. 4 have a very weak dependence on the distance between nanorods.

The Fig.5 shows the dispersion curves have significant differences compared with similar characteristics at Fig. 3 for waveguides with a silver shell, because the complex dielectric constant of gold and silver are essentially different.

## 4. CONCLUSION

For a quantitative estimate the resonant wavelengths of optical nanoantennas should be interpreted them as resonances of double-layer nanowaveguide segments composed of the ZnO core and the thin metal shell excited an integer number of half wavelengths of the waveguide.

The resonances of a periodic waveguide array with average distance between adjacent nanorods 700 nm were presented in paper [1] on wavelengths: 550 nm, 650 nm, 890 nm and 1340 nm. The quantitative estimate calculated by the method described in this paper and by the COMSOL Multiphysics$^{\mathrm{TM}}$ gives values of 500–550 nm, 600–670 nm, 780–800 nm and 1400–1420 nm.

The results discussed in this paper may be used to predict the resonant wavelengths of two-dimensional periodic array of ZnO nanorods grown on a dielectric substrate.

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