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Simulation of Light-Nanowire Interaction in the TE Mode Using Surface Integral Equations

Masoud Rezvani Jalal* and Maryam Fathi Sepahvand

Department of Physics, Malayer University, Malayer, Iran

*Corresponding Author Email: rezvanijalal@malayeru.ac.ir

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ABSTRACT— In this paper, the scattering of a plane monochromatic electromagnetic wave from a nanowire with circular cross-section in the transverse electric (TE) mode is simulated using the well-known Stratton-Chu surface integral equations. For an ordinary dielectric nanowire the refraction phenomenon is nicely simulated. In the case of a plasmonic nanowire no sign of surface plasmon excitation and propagation is seen. Transition from electrostatic regime to the geometrical shadow through diffraction regime by decreasing the light wavelength is also observable.

KEYWORDS: Light-nanowire interaction, Plasmonic nanowire, Stratton-Chu integral, TE mode.

I. INTRODUCTION

Interaction of light with nanostructures is of fundamental importance from both theoretical and experimental points of view [1] and [2]. Many new subfields of nanotechnology such as micro-resonators, nano-plasmonics, photonic molecules, meta-materials, quantum dots, nano-lasers and etc lie in the field of light-nano interaction. Employing the quantum physics and related topics is inevitable to understand the exact mechanism of such interactions and to predict the results or justify the observations. However, in many cases, simple classical models are powerful enough and sufficient to study the interaction. In such cases, the nanostructure is modeled as a dielectric so that its interaction with light can easily be formulated using classical electrodynamics.

Depending on the dielectric function and the geometrical shape of the nanostructure and also the properties of its surrounding medium, the interaction problem can be solved analytically or numerically. Unfortunately, except for few simple configurations, there are no analytical solutions and therefore one should resort to numerical approaches. There are various and robust numerical methods concerning the light scattering from nanostructures. FDTD (Finite Difference Time Domain), DDA (Discrete Dipole Approximation) and SI (Surface Integral) algorithms are among the most famous methods each with its own advantages and drawbacks [3]-[5]. One of the advantages of SI methods is that they deal with lower spatial dimensions than the other volume approaches. Recently, SI methods, especially those based on Stratton-Chu surface integrals, have increasingly been employed to study light-nano interaction. They are really successful in simulating the fine details of the interaction. Using such methods, Rockstuhl *et al.* simulated the scattering of light from a plasmonic nanowire with elliptical cross-section and observed the excitation of localized surface plasmons [6]. Liaw *et al.* also simulated light scattering from various plasmonic nanowire configurations in transverse magnetic (TM) mode by a Stratton-Chu based SI method with Boundary Element Method (BEM) [7] and [8]. They could correctly illustrate the excitation of propagating surface plasmons. However, they did not consider the interaction under TE

mode excitation. Other kinds of integral methods based on the *Green's* function have also been used by other researchers to simulate light-nano interaction [9] and [10].

In the present paper, following the method proposed in Liaw works, light scattering from a nanowire in TE mode is formulated and numerically solved for different nanowires. The paper is organized as follows: In the second section, coupled surface integral equations for TE mode are derived. The third section is devoted to the scattering from a simple and a plasmonic nanowire. Discussions and conclusions are presented in the two last sections.

II. COUPLED SURFACE INTEGRAL EQUATIONS FOR TE MODE

A nanowire with arbitrary cross-section and with homogeneous and isotropic electric permittivity ε_2 and magnetic permeability μ_2 is considered. It is placed in an infinite medium with homogeneous and isotropic electromagnetic constants ε_1 and μ_1 . A plane monochromatic electromagnetic wave with frequency ω is incident on the nanowire whose propagation direction is perpendicular to the wire axis. This is in fact a two-dimensional scattering problem. A cross-sectional cut of the configuration is shown in Fig. 1.

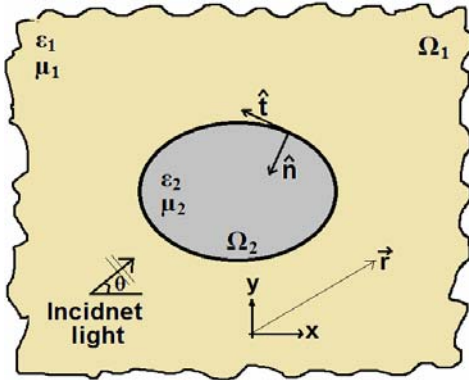


Fig. 1: Cross section of a nanowire (region Ω_2) with ε_2 and μ_2 within an infinite medium (region Ω_1) with ε_1 and μ_1 , irradiated with a electromagnetic plane wave.

The incident light can have any polarization, but, for two special cases the formulation will be simpler: 1) the transverse magnetic (TM) mode in which the magnetic field of incident light is parallel to nanowire axis (here the 'z' axis), and, 2) the transverse electric field (TE) mode that its electric field is set along the nanowire. As mentioned before, the TM case was completely studied in [7] and [8] based on Stratton-Chu surface integral equations. Here, the TE mode with electric field $\mathbf{E}^i(\mathbf{r}) = \hat{\mathbf{e}}_z E_z^i e^{i\mathbf{k}\cdot\mathbf{r}}$ and magnetic induction $\mathbf{B}^i(\mathbf{r}) = (\hat{\mathbf{e}}_x B_x^i + \hat{\mathbf{e}}_y B_y^i) e^{i\mathbf{k}\cdot\mathbf{r}}$ is considered. The superscript 'i' denotes the incident light, $\hat{\mathbf{e}}_x$, $\hat{\mathbf{e}}_y$ and $\hat{\mathbf{e}}_z$ are Cartesian unit vectors and $\mathbf{k} = \hat{\mathbf{e}}_x k_x + \hat{\mathbf{e}}_y k_y$ is the incident wave vector.

In the SI methods, the unknown field values at any point of the space can be calculated from the known values of fields at boundary surfaces present in the problem. For TE mode there are three field unknowns in the space. They are E_z , B_x , and B_y which denote electric field in 'z' direction and magnetic induction in 'x' and 'y' directions, respectively. Based on the Stratton-Chu surface integrals, the fields within the nanowire can be calculated from:

$$\begin{aligned} E_z(\mathbf{r}) &= \int_S E_z(\mathbf{r}') \hat{\mathbf{n}}' \cdot \nabla' G_2(\mathbf{r}, \mathbf{r}') dr' - \\ &\quad i\omega \int_S \mu_2 H_t(\mathbf{r}') G_2(\mathbf{r}, \mathbf{r}') dr' \\ \mathbf{H}(\mathbf{r}) &= -i\omega \int_S \varepsilon_2 G_2(\mathbf{r}, \mathbf{r}') E_z(\mathbf{r}') d\mathbf{r}' + \\ &\quad \frac{1}{\mu_2} \int_S B_n(\mathbf{r}') \nabla' G_2(\mathbf{r}, \mathbf{r}') dr' - \\ &\quad \int_S H_t(\mathbf{r}') \hat{\mathbf{e}}_z \times \nabla' G_2(\mathbf{r}, \mathbf{r}') dr', \quad \mathbf{r} \in \Omega_2 \end{aligned} \quad (1)$$

and the fields out of it from:

$$\begin{aligned} E_z(\mathbf{r}) &= E_z^i(\mathbf{r}) + \int_S E_z(\mathbf{r}') \hat{\mathbf{n}}' \cdot \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' + \\ &\quad i\omega \int_S \mu_1 H_t(\mathbf{r}') G_1(\mathbf{r}, \mathbf{r}') dr' \end{aligned}$$

$$\begin{aligned} \mathbf{H}(\mathbf{r}) = & \mathbf{H}^i(\mathbf{r}) + i\omega \int_S \varepsilon_1 G_1(\mathbf{r}, \mathbf{r}') E_z(\mathbf{r}') \vec{d}\mathbf{r}' + \\ & \frac{1}{\mu_1} \int_S B_n(\mathbf{r}') \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' - \\ & \int_S H_t(\mathbf{r}') \hat{\mathbf{e}}_z \times \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' \quad , \quad \mathbf{r} \in \Omega_1 \end{aligned} \quad (2)$$

where $\hat{\mathbf{n}}$, H_t , and B_n are normal unit vector, tangential component of magnetic field and normal component of magnetic induction at the nanowire surface S , respectively. G_1 and G_2 are Green's functions for the surrounding medium and the nanowire, respectively:

$$G_j(\mathbf{r}, \mathbf{r}') = \frac{i}{4} H_0^{(1)}(k_j |\mathbf{r} - \mathbf{r}'|) \quad , \quad j = 1, 2 \quad (3)$$

where $H_0^{(1)}$ is the zero order Hankel's function of the first kind and $k_j = \omega \sqrt{\varepsilon_j \mu_j}$ is the wave number. If the observation point approaches the boundary surface from both interior and exterior regions then Eqs. (1) and (2) yield:

$$\begin{aligned} \frac{1}{2} E_z(\mathbf{r}) = & \int_S E_z(\mathbf{r}') \hat{\mathbf{n}}' \cdot \nabla' G_2(\mathbf{r}, \mathbf{r}') dr' - \\ & i\omega \int_S \mu_2 H_t(\mathbf{r}') G_2(\mathbf{r}, \mathbf{r}') dr' \\ \frac{1}{2} \mathbf{H}(\mathbf{r}) = & -i\omega \int_S \varepsilon_2 \mathbf{G}_2(\mathbf{r}, \mathbf{r}') E_z(\mathbf{r}') \vec{d}\mathbf{r}' + \\ & \frac{1}{\mu_2} \int_S B_n(\mathbf{r}') \nabla' G_2(\mathbf{r}, \mathbf{r}') dr' - \\ & \int_S H_t(\mathbf{r}') \hat{\mathbf{e}}_z \times \nabla' G_2(\mathbf{r}, \mathbf{r}') dr' \quad , \quad \mathbf{r} \in S \end{aligned} \quad (4)$$

and:

$$\begin{aligned} \frac{1}{2} E_z(\mathbf{r}) = & E_z^i(\mathbf{r}) + \\ & \int_S E_z(\mathbf{r}') \hat{\mathbf{n}}' \cdot \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' + \\ & i\omega \int_S \mu_1 H_t(\mathbf{r}') G_1(\mathbf{r}, \mathbf{r}') dr' \end{aligned}$$

$$\begin{aligned} \frac{1}{2} \mathbf{H}(\mathbf{r}) = & \mathbf{H}^i(\mathbf{r}) + i\omega \int_S \varepsilon_1 G_1(\mathbf{r}, \mathbf{r}') E_z(\mathbf{r}') \mathbf{d}\mathbf{r}' + \\ & \frac{1}{\mu_1} \int_S B_n(\mathbf{r}') \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' - \\ & \int_S H_t(\mathbf{r}') \hat{\mathbf{e}}_z \times \nabla' G_1(\mathbf{r}, \mathbf{r}') dr' \quad , \quad \mathbf{r} \in S \end{aligned} \quad (5)$$

In Eqs. (4) and (5) \mathbf{r} and \mathbf{r}' are respectively the observation point and the integration variable both located at the nanowire surface. Equating tangential component of \mathbf{E} , tangential component of \mathbf{H} and normal component of \mathbf{B} from the interior and the exterior formulae at the surface, yields the following coupled surface integral equations:

$$\begin{aligned} E_z(\mathbf{r}) = & E_z^i(\mathbf{r}) - \int_S E_z(\mathbf{r}') \hat{\mathbf{n}}' \cdot \nabla' [G_1 - G_2] dr' + \\ & i\omega \int_S [\mu_1 G_1 - \mu_2 G_2] H_t(\mathbf{r}') dr' \quad , \\ B_n(\mathbf{r}) = & B_n^i(\mathbf{r}) + \\ & i\omega \int_S E_z(\mathbf{r}') [\mu_1 \varepsilon_1 G_1 - \mu_2 \varepsilon_2 G_2] \hat{\mathbf{n}} \cdot \mathbf{d}\mathbf{r}' - \\ & \int_S B_n(\mathbf{r}') \hat{\mathbf{n}} \cdot \nabla' [G_1 - G_2] dr' + \\ & \int_S H_t(\mathbf{r}') \hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_z \times \nabla' [\varepsilon_1 G_1 - \varepsilon_2 G_2] dr' \quad , \\ H_t(\mathbf{r}) = & H_t^i(\mathbf{r}) + \\ & i\omega \int_S E_z(\mathbf{r}') [\varepsilon_1 G_1 - \varepsilon_2 G_2] \hat{\mathbf{t}} \cdot \mathbf{d}\mathbf{r}' - \\ & \int_S B_n(\mathbf{r}') \hat{\mathbf{t}} \cdot \nabla' \left[\frac{G_1}{\varepsilon_1} - \frac{G_2}{\varepsilon_2} \right] dr + \\ & \int_S E_t(\mathbf{r}') \hat{\mathbf{t}} \cdot \hat{\mathbf{e}}_z \times \nabla' [G_1 - G_2] dr' \quad , \end{aligned} \quad (6)$$

in which $\hat{\mathbf{t}} = \hat{\mathbf{n}} \times \hat{\mathbf{e}}_z$ is the tangential unit vector at the surface. Eq. (6) contains three coupled surface integral equations of Fredholm second kind that govern E_z , B_n , and H_t at the boundary surface. Their form is similar to the coupled surface integral equations derived for TM mode (containing H_z , D_n , and E_t) in [7] and [8] but with interchanged role of ε and η . Such coupled integral equations do not have, in general, analytical solutions and should be numerically solved.

III. NUMERICAL SOLUTION

In order to solve the coupled integral equations in Eq. (6), the simplest trapezoidal integration scheme is used. First, the boundary is divided into N segments. At each segment there are three unknown fields, namely, E_z , B_n and H_t which are related to each other through coupled integrals in Eq. (6). The discretized form of Eq. (6) is constructed as:

$$\begin{aligned}
E_z(p) &= E_z^i(p) - \sum_{q=1}^N a(p,q) E_z(q) + \\
&\quad \sum_{q=1}^N b(p,q) H_t(q), \\
B_n(p) &= B_n^i(p) + \sum_{q=1}^N c(p,q) E_z(q) + \\
&\quad \sum_{q=1}^N d(p,q) B_n(q) + \\
&\quad \sum_{q=1}^N e(p,q) H_t(q), \\
H_t(p) &= H_t^i(p) + \sum_{q=1}^N f(p,q) E_z(q) + \\
&\quad \sum_{q=1}^N g(p,q) B_n(q) + \\
&\quad \sum_{q=1}^N h(p,q) H_t(q), \tag{7}
\end{aligned}$$

where p and q are p^{th} and q^{th} segments of the boundary, respectively. The functions $a(p,q)$ to $h(p,q)$ are coefficients of the unknown fields and can easily be derived from Eq. (6) as:

$$\begin{aligned}
a(p,q) &= -\hat{\mathbf{n}}(q) \cdot \nabla_q [G_1(p,q) - G_2(p,q)] \Delta l_q, \\
b(p,q) &= i\omega [\mu_1 G_1(p,q) - \mu_2 G_2(p,q)] \Delta l_q, \\
c(p,q) &= i\omega [\mu_1 \varepsilon_1 G_1(p,q) - \mu_2 \varepsilon_2 G_2(p,q)] \hat{\mathbf{n}}(p) \cdot \hat{\mathbf{t}}(q) \Delta l_q, \\
d(p,q) &= -\hat{\mathbf{n}}(p) \cdot \nabla_q [G_1(p,q) - G_2(p,q)] \Delta l_q, \\
e(p,q) &= \hat{\mathbf{n}}(p) \cdot \hat{\mathbf{e}}_z \times \nabla_q [\varepsilon_1 G_1(p,q) - \varepsilon_2 G_2(p,q)] \Delta l_q, \\
f(p,q) &= i\omega [\varepsilon_1 G_1(p,q) - \varepsilon_2 G_2(p,q)] \hat{\mathbf{t}}(p) \cdot \hat{\mathbf{t}}(q) \Delta l_q, \\
g(p,q) &= -\hat{\mathbf{t}}(p) \cdot \nabla_q \left[\frac{G_1(p,q)}{\varepsilon_1} - \frac{G_2(p,q)}{\varepsilon_2} \right] \Delta l_q, \\
h(p,q) &= \hat{\mathbf{t}}(p) \cdot \hat{\mathbf{e}}_z \times \nabla_q [G_1(p,q) - G_2(p,q)] \Delta l_q. \tag{8}
\end{aligned}$$

with Δl_q as the length of the q^{th} segment. All of the above coefficients are well-defined for $p \neq q$. However, denominator of the Green's functions and their derivatives vanish for $p=q$ case which will be problematic. Using the

trick of Cauchy principal value shows that all the coefficients vanish at limits $q \rightarrow p$ and $\Delta l_q \rightarrow 0$ except for $b(p,q)$ and $f(p,q)$. They are determined to have the following limits:

$$\begin{aligned}
\lim_{q \rightarrow p} b(p,q) &= \\
& i\omega [\mu_1 G_1(p,p+1) - \mu_2 G_2(p,p+1)] \Delta l_p, \\
\lim_{q \rightarrow p} f(p,q) &= \\
& i\omega [\varepsilon_1 G_1(p,p+1) - \varepsilon_2 G_2(p,p+1)] \hat{\mathbf{t}}(p) \cdot \hat{\mathbf{t}}(p+1) \Delta l_p, \tag{9}
\end{aligned}$$

With these coefficients in hand, the Eq. (7) yields three non-homogenous linear algebraic equations for each segment. Consequently, for N segments there are $3N$ non-homogenous equations with $3N$ unknowns. They can be solved simply by matrix algebra. Using the found fields at the boundary, the other field values within the nanowire and surrounding medium can be calculated through Eqs. (1) and (2), respectively. Integral equations in Eqs. (1) and (2) are normal and can be implemented easily by a simple trapezoidal scheme with no need to Cauchy principal value or other tricks.

To do the calculations, a massive computer code was developed by the authors. All of the mentioned procedures including boundary discretization, coefficients evaluation, matrix manipulation and field computation are automatically done by the code. In the following subsections two examples are presented.

A. Interaction with an ordinary dielectric nanowire

A simple dielectric nanowire (here a glass) with circular cross-section of radius $R=400$ nm and with $\varepsilon_2=2.25 \varepsilon_0$ and $\mu_2=\mu_0$ is considered. The nanowire is placed in the vacuum and is illuminated by a TE-polarized plane wave with wavelength $\lambda=400$ nm. The interaction of light with the nanowire is simulated by the mentioned code. A square region of side length 800 nm with the nanowire in its center is considered as the computational space and is divided into differential squares of side length 5 nm. The nanowire boundary is discretized

into $N=500$ segments. Simulated distribution of E_z^2 is shown in Fig. 2a for a typical time.

Fig. 2a clearly shows that in this interaction, the incident light is refracted with a smaller wavelength within the wire (because $\epsilon_2 > \epsilon_1$) and transmits (forward-scattered) through it. The transmitted light is focused in a point within the vacuum confirming the fact that it acts as a cylindrical lens. A portion of the light is also reflected (back-scattered) from the nanowire and interferes with the incident field and constructs an interference pattern.

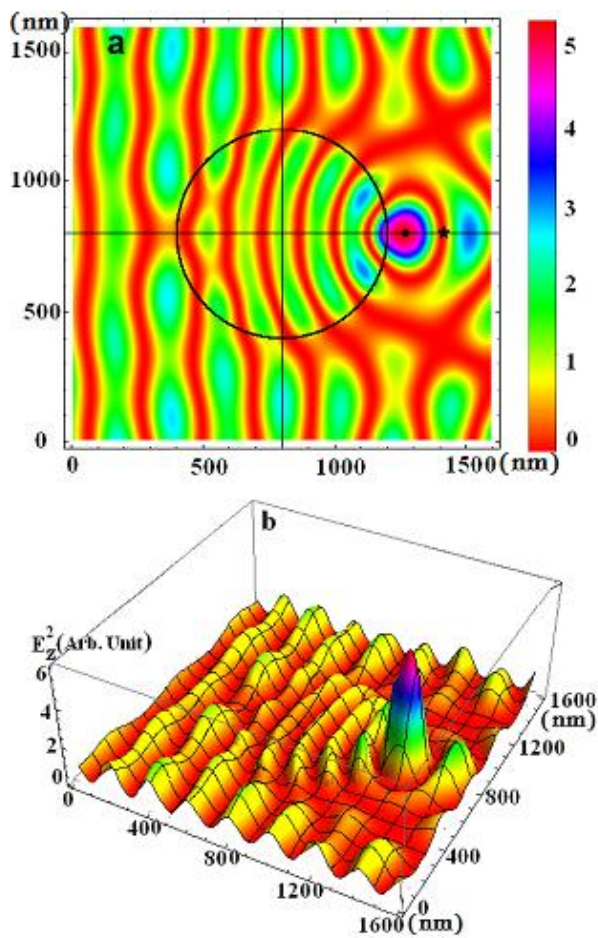


Fig. 2: Contour plot of simulated E_z^2 in scattering of a plane TE polarized light from a glass nanowire, a. The three-dimensional plot of such distribution, b.

B. Interaction with a plasmonic nanowire

In this subsection, a silver nanowire with circular cross-section of radius $R=400$ nm is considered. The nanowire is placed in the vacuum and is interacted by a TE polarized

light with $\lambda=400$ nm. The electromagnetic constants of silver in $\lambda=400$ nm, as reported in [7], are $\epsilon_2=\epsilon_0 (-4.22+i0.73)$ and $\mu_2=\mu_0$, respectively. In this wavelength, silver is a plasmonic material and can support surface plasmon wave under interaction with a TM polarized light.

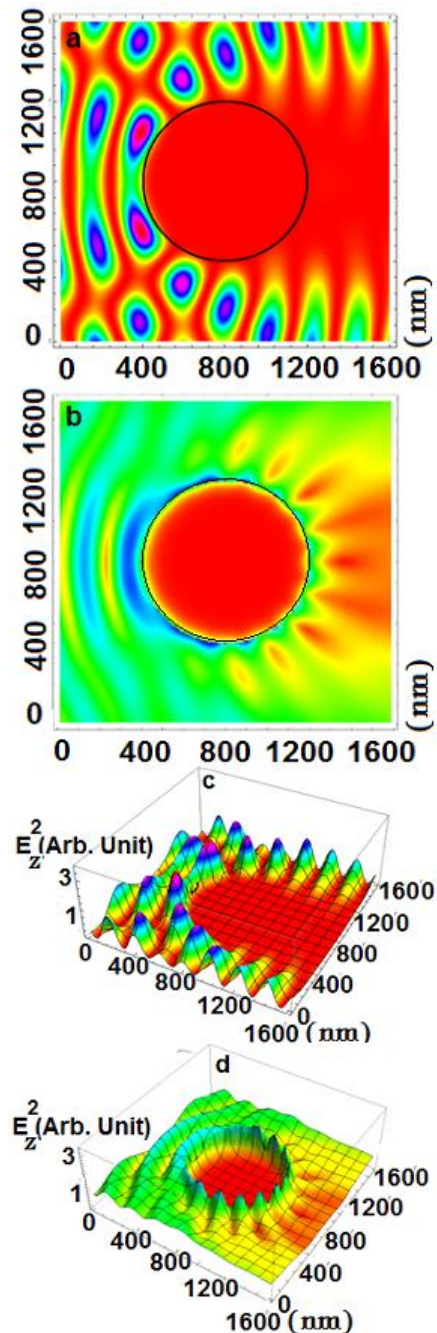


Fig. 3: Contour plot of the simulated E_z^2 in scattering of a plane TE polarized light from a plasmonic nanowire, a, and its three dimensional plot, c. The same plots for scattering of a TM polarized light from a plasmonic nanowire, b and d.

The simulated distribution of E_z^2 in contour and three-dimensional plots is shown in Figs. 3a and 3c, respectively. It is seen that no electric field penetrates into the nanowire. This is due to the imaginary part of ϵ_2 representing a kind of loss mechanism. The transmitted light is vanishingly zero but the reflected one is significant; confirming the fact that silver is a good reflector of light.

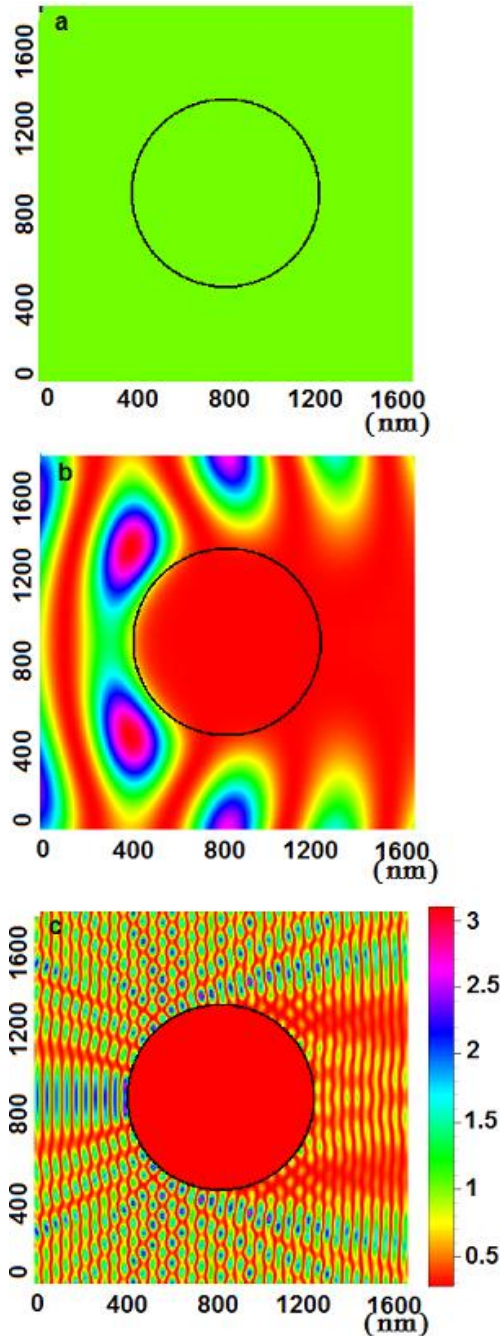


Fig. 4: Contour plots of the field distribution in scattering of a plane TE-polarized light from a plasmonic nanowire for $\lambda \gg R$, a, for $\lambda \approx 2R$, b, and for $\lambda \ll R$, c.

In the surface region, there is no sign of surface plasmon excitation and propagation. If the incident light was in TM mode rather than in TE, then surface plasmon would be excited and propagate at the surface. This mode was also calculated by the code and its results are plotted in Figs. 3b and 3d showing the excitation and propagation of surface plasmons. The figures show that, excitation of propagating surface plasmon by TM mode can guide the incident light to the dark back region of the wire and lighten there, but, there is no such thing in the TE mode. More details of TM mode scattering can be found in [7] and [8].

Field distributions for very large wavelengths ($\lambda \gg R$), for moderate wavelengths ($\lambda \approx 2R$), and very small wavelengths ($\lambda \ll R$) are calculated by the code and plotted in Figs. 4a, 4b and 4c, respectively. At $\lambda \gg R$ extreme, which is the electrostatic limit, the electric field penetrates through the whole of nanowire. In this limit there is no sign of reflected and transmitted light and also no dark region (shadow) behind it. For $\lambda \approx 2R$ case a pattern which contains spatial distribution of minima and maxima is formed. The pattern is in fact the familiar light diffraction from the wire. A shadow-like dark region is being constructed in its back. For the other extreme $\lambda \ll R$, the incident light on the wire is completely reflected from the wire and the geometrical shadow is formed behind it.

IV. DISCUSSION

Simulation of light scattering from a glass nanowire correctly shows light reflection, refraction with a smaller wavelength, transmission and also its concentration in a focus which reminds that it is a cylindrical lens. In geometrical optics the focal length of a thick lens in air is calculated from [11]:

$$\frac{1}{f} = (n_l - 1) \left(\frac{1}{R_1} - \frac{1}{R_2} + \frac{(n_l - 1)d}{n_l R_1 R_2} \right) \quad (10)$$

where n_l is the lens refractive index, R_1 and R_2 are curvature radii of left and right surfaces of the lens, respectively, and d is the lens

thickness. For the cylindrical scatterer of Fig. 2, which is in fact a thick glass lens, the focal point is calculated to be 600 nm on the right of the wire center. Its position is shown by a small star in Fig. 2. This position is different from the simulated focus shown by a small point in the figure. The origin of the difference is the fact that the Eq. (10) is derived in geometrical optics (i.e. short wavelengths compared to the lens size) by paraxial approximation. In the Stratton-Chu integral equations mentioned above no such approximations were applied and the results are exact.

In the scattering of the TE light from a plasmonic nanowire no sign of plasmon excitation and propagation is seen. It is different from the TM light scattering in which surface plasmon is excitable. Surface plasmon is an electronic wave that can be excited in material surfaces by incident light whenever two necessary conditions are satisfied [12]. The first condition is that the real part of electric permittivity of the material (ϵ_{2r}) must have different sign from that of the surrounding medium (ϵ_{1r}). The second condition is that there must be a normal component of electric field on the surface. In the scattering of TE light from silver nanowire the first condition is satisfied. However, as the electric field of TE mode is parallel with the wire axis it does not have normal component on the nanowire surface and so the second condition is not satisfied.

Light scattering with decreasing wavelengths shows that the electrostatic, diffraction and geometrical optics regions appear in turn. This result is discussable from two aspects. Firstly, for very long wavelengths (compared to scatterer size), no scattering will occur and the incident light will propagate unperturbedly. In fact, small objects will not scatter long-wavelength lights, or in other words, a long-wavelength light cannot see small objects. Secondly, if wavelength of the incident light is comparable to size of the scatterer then diffraction occurs. Diffraction is a direct result of wave-like nature of the light. By decreasing

the wavelength of the incident light the diffraction level also decreases. In fact, the geometrical optics is the sort-wavelength limit of the wave optics with zero diffraction and with distinct shadow regions.

V. CONCLUSION

In this paper, three coupled surface integral equations governing the scattering of a monochromatic TE polarized light from a nanowire were derived. The simulation results for different nanowires and their physical interpretation show that the derived equations are correct and powerful. Extension to the scattering of a TE polychromatic light is considered as the future work of the authors.

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Masoud Rezvani Jalal was born in Lalejin of Hamedan in 1980. He received his BSc. from Razi University, his MSc. from Tarbiat Modarres University, and his PhD. from

University of Tehran in 2002, 2005, and 2010, respectively.

He has academic skills in atomic and molecular physics in the fields of lasers, optics, and plasmas. He is a member of faculty in physics department of Malayer University.



Maryam Fathi Sepahvand was born in Khorram Abad of Lorestan in 1989. She received her BSc. and MSc. from Islamic Azad University of Khorramabad and Malayer University in 2012 and 2014, respectively. She has a high level of skills in computational physics in the field of nano-photonics especially nano-plasmonics.

She is working on a research project about computational nano-plasmonic in cooperation with Malayer University.

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