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Simulation of Surface Plasmon Excitation in a Plasmonic Nano-Wire Using Surface Integral Equations

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Abstract: In this paper, scattering of a plane and monochromatic electromagnetic wave from a nano-wire is simulated using surface integral equations. First, integral equationsgoverning unknown fields on the surface is obtained based on Stratton-Cho surface integral equations. Then, the interaction of the wave with a non-plasmonic as well as a palsmonic nano-wire is considered. It is shown that in scattering of the wave from the non-plasmonic nano-wire the simple phenomena of refraction and transmission occur. On the other hand, the interaction of TM polarized light with plasmonic nano-wire excites surface plasmon waves. Simulations show that no surface plasmon is excited in interaction of TE polarized light with plasmonioc nano-wire. It is observed that, while increasing the frequency of incident light, the regime of scattering goes from electrostatic limit to simple geometric limit through diffraction region. In continuation, charge distribution induced by surface plasmon is simulated for different times. The simulation shows that a wave-like surface charge is excited and propagates on the surface.There is a very weak charge distribution within the nano-wire indicating that no light penetrates the wire.

Keywords: light scattering of nanowires, surface integral equations stratton-chu, surface plasmon.

1. Introduction

Surface plasmons are collective oscillations of electrons in the metal-dielectric interface [1, 2]. This oscillation occurs when metallic nanoparticles are exposed to lightwith a wavelengthappropriately [1, 3-5]. When thefrequency of the incident lighton the nanoparticle is equal tosurface Plasmon frequency resonance phenomena happens. Thereseononcefrequency depends onconfiguration, size, material, and media dielectric [6-8]. Whensurface Plasmon resonance in ametallic nanoparticle occurs, stronglocalelectric fieldsaround theparticle iscreatedwhich this fieldcan bemuch stronger thanthe electric field of incidentlight [1,9]. This local strong field is used in the

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manufacture of biological andchemical sensors, single-molecule detection, nano-lens, nano-antennas, high power devices, p-n junctions, and surfaceenhancedRaman scattering (SERS) [10-17].

Analytical study of surface Plasmon excitation and propagation in metal nanoparticles mostly are limited to spherical nanoparticles. The Mie theory [18-20] that uses spherical harmonic [21-24] is in this category of studies.Along with analytical methods, there are strongnumerical methods, which are not limited to a specific shape of nanoparticles. Finite different time domain (FDTD) [25,26], discrete dipole approximation (DDA) and surface integral equations (SIE) are the most well-known of the numerical methods for the simulation of light scattering [27]. Of course, these numerical methods have some limitations. For example, the disadvantage of FDTD method is the dependence of its accuracy on the number of elements, so that to simulation of the near fields effects (for example, the field distribution close to nano-particles), a dense element mesh is needed that is led to increase of calculations. DDA approximates a continuous matterby an array of dielectric dipoles.In this method to achieve an appropriate accuracy, very high volumes of computations and computer resources is needed.

The surface integral method, because of the geometrical dimensions of the problem can be diminished the speed and accuracy of calculations are high. The method is ideal especially in near-field calculation.Surface integral method is based on the so-called Stratton-Chu integral equations and yields field at any point in space by known fieldson the surface [28-31].

In this paper,using theStratton-Chu integral equations, integral equationscontaining thefields in the border of the nanowires are obtained. Then,the equationsofFredhelminthesgral equationsofthe second kindforplasmonicand non-plasmonic nanowireswith acircularcross sectionare numericallysolvedandthe unknownfieldsarespecifiedin thenanono wires. Having the fieldsinthe boundarythe field distribution in the whole space is calculated and the scattering problem is simulated.

2. Surface integral equations

A plasmonic material with axial symmetry is considered in a uniform infinite medium. The configuration is shown in Fig. 1.

This configuration is essentially a two-dimensional configuration with symmetry about z axis. In this configuration, a plane electromagnetic wave is incident with the shown angle. TM polarization of the incident light is a polarization in which the magnetic field is in the z-axis and the electric field in the x-y plane. Electric field of such a polarization is $E=E_x e_x+E_y e_y$ and its magnetic is $H=H_z e_z$ .E and H fields are coupled equations in Ω_2 region through Stratton-Chu Ω_2 as follows [28-30]:

$$\begin{aligned} H_z(\vec{r}) &= \int_S H_z(\vec{r}\,')\hat{\mathbf{n}}'.\vec{\nabla}' G_2 dl' + i\omega \int_S \varepsilon_2 E_t(\vec{r}\,') G_2 dl', \\ \vec{\mathbf{E}}(\vec{r}) &= i\omega \int_S \mu_2 \mathbf{G_2} H_z(\vec{r}\,') d\vec{\mathbf{l}}' + \frac{1}{\varepsilon_2}\int_S D_n(\vec{r}\,')\vec{\nabla}' G_2 dl' - \int_S E_t(\vec{r}\,')\hat{\mathbf{e}}_{\mathbf{z}} \times \vec{\nabla}' G_2 dl' \end{aligned} \tag{1}$$

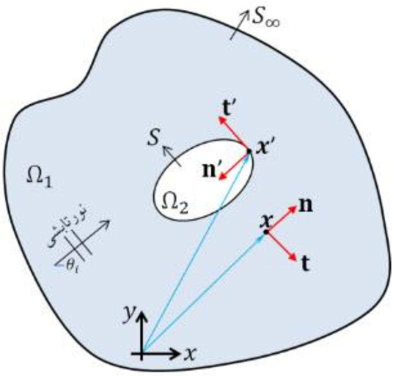

Fig. 1. The scheme of the two-dimensional problem.

Electric field and magnetic field in the area $\Omega_1$can be divided into two parts, namely the $E=E^i+E^s$ and $H=H^i+H^s$, where the letters i and s represent the incident and the scattered parts, respectively. The time response is considered to be harmonic harmonic $e^{-i\omega t}$. Field distribution in Ω_1 section reads:

$$\begin{aligned} H_z^s(\vec{r}) &= \int_S H_z^s(\vec{r}\,')\hat{\mathbf{n}}'.\vec{\nabla}' G_1 dl' - i\omega \int_S \varepsilon_1 E_t^s(\vec{r}\,') G_1 dl' \\ \vec{\mathbf{E}}^s(\vec{r}) &= -i\omega \int_S \mu_1 G_1 H_z^s(\vec{r}\,') d\vec{\mathbf{l}}' + \frac{1}{\varepsilon_1}\int_S D_n^s(\vec{r}\,')\vec{\nabla}' G_1 dl' - \int_S E_t^s(\vec{r}\,')\hat{\mathbf{e}}_{\mathbf{z}} \times \vec{\nabla}' G_1 dl' \end{aligned} \tag{2}$$

In Eqs. 1 and 2, ε is dielectric coefficient and μ is the permeability coefficient.ω is angular frequency of the incident light, S represents the border of the nanowires, $r' \in S$ .n/ the normal vector on the border, and e_z unit vector in the direction of the axis z. H_z, D_n and E_t are axial magnetic field, displacement field perpendicular to the surface and the tangential electric field at the surface, respectively. Green function which issingular response of the Helmholtz equation, must satisfy the following equation(j=1, 2):

$$\nabla^2 G_j + \omega^2 \varepsilon_j \mu_j G_j = -\delta(\mathbf{x} - \mathbf{x}') \tag{3}$$

with:

$$G_j(\mathbf{x}', \mathbf{x}) = \frac{i}{4} H_0^{(1)}(k_j \,|\, \mathbf{x} - \mathbf{x}' \,|) \tag{4}$$

Where $H_0^{(1)}$ is the Hankel function of the first kind of order zero, and $k_j = \omega\sqrt{\varepsilon_j\mu_j}$. Writing Eqs. 1 and 2 fornanowires surface and doing some calculations, the following integral equations are obtained:

$$
\begin{aligned}
H_z(\vec{r}) &= H_z^i(\vec{r}) - \int_S H_z(\vec{r}\,')\hat{\mathbf{n}}'.\vec{\nabla}'\left[G_1 - G_2\right]dl' - i\omega\int_S \ \varepsilon_1 G_1 - \varepsilon_2 G_2 \ \ E_t(\vec{r}\,')dl',\\
D_n(\vec{r}) &= D_n^i(\vec{r}) - i\omega\int_S H_z(\vec{r}\,')\left[\varepsilon_1\mu_1 G_1 - \varepsilon_2\mu_2 G_2\right]\hat{\mathbf{n}}\cdot \vec{\mathrm{d}}\mathbf{l}'\\
&\quad -\int_S D_n(\vec{r}\,')\hat{\mathbf{n}}\cdot\vec{\nabla}'\left[G_1 - G_2\right]dl' + \int_S E_t(\vec{r}\,')\hat{\mathbf{n}}\cdot\hat{\mathbf{e}}_z\times\vec{\nabla}'\left[\varepsilon_1 G_1 - \varepsilon_2 G_2\right]dl',\\
E_t(\vec{r}) &= E_t^i(\vec{r}) - i\omega\int_S H_z(\vec{r}\,')[\mu_1 G_1 - \mu_2 G_2]\hat{\mathbf{t}}\cdot\vec{\mathrm{d}}\mathbf{l}'\\
&\quad -\int_S D_n(\vec{r}\,')\hat{\mathbf{t}}\cdot\vec{\nabla}'\left[\frac{G_1}{\varepsilon_1} - \frac{G_2}{\varepsilon_2}\right]dl + \int_S E_t(\vec{r}\,')\hat{\mathbf{t}}\cdot\hat{\mathbf{e}}_z\times\vec{\nabla}'\left[G_1 - G_2\right]dl'
\end{aligned}
\tag{5}
$$

Where $\vec{r}$ and $\vec{r}\,'$ are two pointson theboundary ofnano-wires. Eqs. 5 areFredholm integral equations of the second kind [32]. In this paper, the integration is done by a simple trapezoidal algorithm and to overcome the singularity of the Green's function in the kernel integral equations, Cauchy principal value is used.

3. Numerical approach

As mentioned in the introduction surface plasmon onmetalnano particles can be created. In fact, a necessary condition for the formation ofsurfaceplasmon is that the real part of the dielectric coefficient of the particle be opposite to that of the surrounding medium. For noble metals (such as gold and silver) real part of the dielectric coefficient is negative and when the metal in the visible spectrum is placed in a conventional dielectric such as the air then surface plasmon resonance condition is easily met. Therefore, these metals are usually called plasmonic materials. In the first part, a non-plasmonic materials (such as glass) is irradiated by an incident light with TM polarization. In the second part, a plasmonic matter is irradiated with both TM and TE polarizations. For different wavelengths, field distribution within and around the nanowires is also calculated.

In all simulations, a nanowire with circular section of radiusR= 400 nm is used. A massive Mathematical code is developed by the authors for calculations. This code first discretizes the nano-wire surface to 800 nodes.Then, unknown fields H_z, D_n, andE_t in each node is calculated by solving integral Eqs. 5 with trapezoidal integration and matrix algebra. This code after obtaining the unknown fields on the border, using integral Eqs. 1 and 2 calculates other fields inside and outside of the nanowires. All of simulations conducted in this study aredone by a 64-bit computer with 8 GB of internal memory (RAM) CPU 2/2 GHz with model ofIntel ® Core ™ i7-4702MQ.

3-1-Simulation of light scattering of non-plasmonic nanowires

Here, scattering of TM light from a non-plasmonic materials such as glass with dielectric coefficient $\varepsilon_2=2.5\ \varepsilon_0$in the air $\varepsilon_1 = \varepsilon_0$, is simulated. The simulation results are shown in Fig. 2.As expected, no effect of surface plasmon excitation is not seen on the nanowire and only the simple phenomenon refraction occurs inside nanowire.Lack of surface plasmon excitation can be attributed to the iso-sign of real parts of dielectric constants.The same results were obtained for the scattering of light by the polarization TE but not shown here. The simulation time in this case is 1093 min.

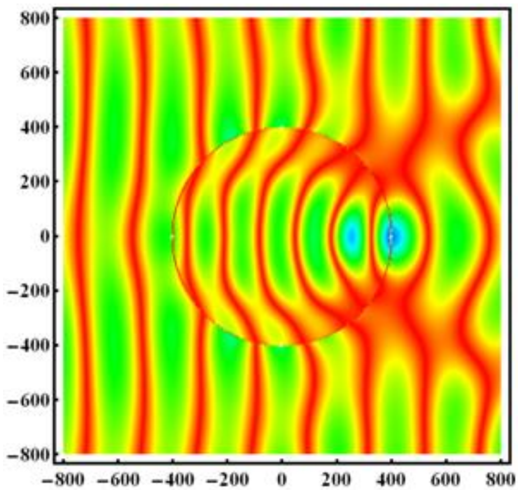

Fig. 2. Distribution of the electric field in and around a non-plasmonic nanowires under light with polarization TM (axes unit is nano-meters).

3-2-TE polarized light scattering from plasmonic nanowires

In this section, as in the previous section, the mechanism of formation of plasmons is studied with this difference that the non-plasmonic material is replaced with a plasmonic one. Since the TM polarized light scattering integral equations is obtained with Eqs. 5 similar equations can be derived for TE light. TE polarization as TM polarization has three field components two for the magnetic field and onefor the electric field ($H=H_xe_x+H_ye_y$ and $E=E_ze_z$). Equations of TE polarization aresimilar to that of TM polarization in the Eqs.1, 2 and 5with the difference that H, E, D, ε and μ, should be replaced with E, H, B, μ and ε, respectively. Silver is a plasmonic material with dielectric coefficient$\varepsilon_2=\varepsilon_0(-4.42 +0.73i)$ [30]. Through simulation, the field distribution is obtained and is shown in Fig. 3. In Fig. 3-a real part of the electric field distribution and in Fig. 3-b its absolute value is given. As you can see, there is still no sign of a strong electric field of surface plasmon oscillations near the surface of the nanowires.The reason for this can be attributed to the fact that no plasmon excitation occurs under TE polarization.

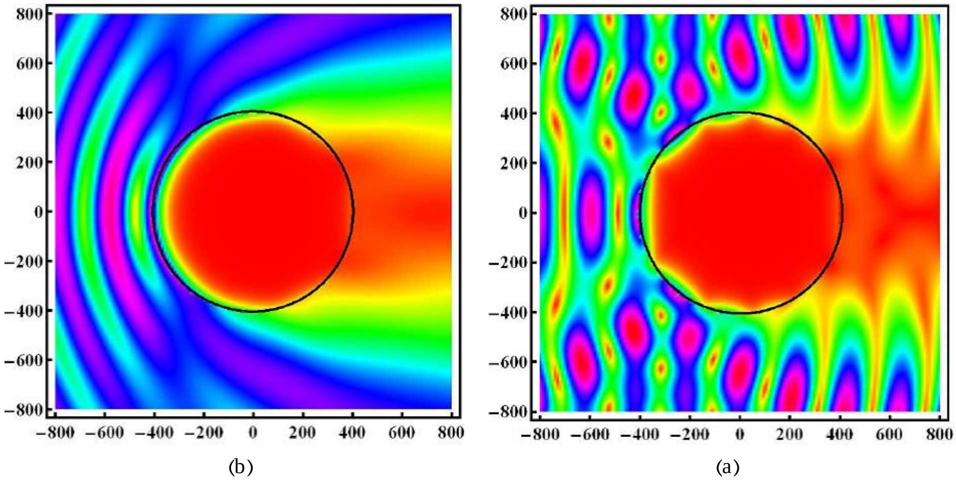

Fig. 3. TE polarized light scattering from a plasmonic nanowire,(a) the real part of the electric field, (b) the size distribution of the absolute value of the electric field (axes unit is nano-meter).

3-3-TM polarized light scattering from a plasmonic nanowire

Simulations showed that in the previous two light scattering problems with non-plasmonic materials and with a plasmonic material under TE irradiation no surface plasmon is created. In this section, field distribution in a plasmonic nanowire under light with TM polarization and with different wavelengths is simulated. Plasmonic material considered here, as in the previous section, is silver. Since the purpose of this section is merely to evaluate the formation of surface plasmon on the surface of a plasmonic material soany dispersion is ignored. The result of simulations of the scattering of the incident light with different wavelengths ($\lambda >> R$, $\lambda = R$ and $\lambda << R$) is shown in Fig. 4. Fig. 4-a is distribution of the absolute value of the electric field. Fig. 4-b is field lines of real part of the electric field. The electric charge density distribution is shown in Fig. 4-c.According to this figure, much information can be inferred:

1) For $\lambda >> R$ which is electrostatic limit, a strong electric field is formed at the top and the bottom of the wire.A localized surface plasmon excitation is visible. In this mode, no sign ofgeometric shadow or light scattering is seen behind the nanowire. The charge distribution is reminiscent of an electric dipole with positive charge at the top and

negative one at the bottom.Charge density within the nanowirehas values close to zero due to the lack of penetration of the radiation into the nanowire.

2) For λ=R, a propagating surface plasmon can be seen on the surface of the nanowire. In back side of the nanowire also the sign of diffraction pattern with bright and dark areas is clearly seen. In this mode the electric field lines behave similar to a multi-polefield. Charge density distribution within the nanowire is zero, but at the nanowire surface a periodic distribution of positive and negative surface charge is created.
3) For λ<<R there is no surface plasmon and the effects of light scattering is eliminated and instead a clear geometric shadow behind the nanowire is created. In this mode also a periodic surface charge density near the surface is created butits value is very low and weak and the positive and negative charges seen very close to each other.A very weak field line inside the nanowires confirms that no electric field penetrates into the nanowire.

It is worth mentioning that the temporal evolution of charge distribution in any point of the space inside and outside the nanowire can be calculated from $\rho = \varepsilon \vec{\nabla}.\vec{E}$. This distribution is calculated using mentioned code through a finite difference method as follows:

$$\rho = \varepsilon \left[\frac{E_x\ i+1, j\ - E_x\ i-1, j}{2\Delta x} + \frac{E_y\ i, j+1\ - E_y\ i, j-1}{2\Delta y} \right] \tag{6}$$

where Δx and Δy are spatial divisions of computational space.

3-4-TM light scattering in different times

In this section, the temporal evolution ofthedistributionandensity from scattering of TM light from a silver nanowire at wavelengthλ≈R=400nm is simulated. This wavelength is almost equal to the resonant wavelength of thesurface plasmon in silver [30]. Field distributionforfivedifferent time is = 0, t = 0.25T, t = 0.5T, t = 0.75T and t = T is simulatedwhere Tis theperiod ofthe incidentlight. The results of the simulation are shown in Fig. 5. Fig. 5-ais distribution of the real part of the electric field and Fig. 5-b is field lines of the real part of the electric field.Electric charge density distribution is shown in Fig. 5-c. The two parallel linesindicate thewidth ofawavelengthλ.Simulationruntimes from 0 toTare991,987, 996, 986and975minutes, respectively.

Ascan be seenfrom Fig. 5, the field distributionfor thetimet = 0andt = Tisexactly the same. At times t = 0.25 T and T = 0.75 T the distribution of the size of the real part of the electric field are identical but with opposite directions of electric fields. The same situation is evident for t = 0 (or t = T) and t = 0.5 T. Charge density distribution in Fig. 5-cfor all timesis non-zero on the surface but the density inside of the nanowire is almost zero.

In Fig. 6, the plot of the surface charge density for different times is drawn. Surface charge density is obtained from σ = D.nrelation. Asis clear from Fig. 6thecharge curveat = 0 (or t = T) is opposite to t = 0.5 T. Times t = 0.25 Tandt = 0.75 T have the same situation. Fig. 6-b which is the magnified vision of time t = 0, shows the direction of polarizationof lightthatisperpendicular to the directionof light propagation. One can use the diagrams to find the speed of surface plasmon wave.

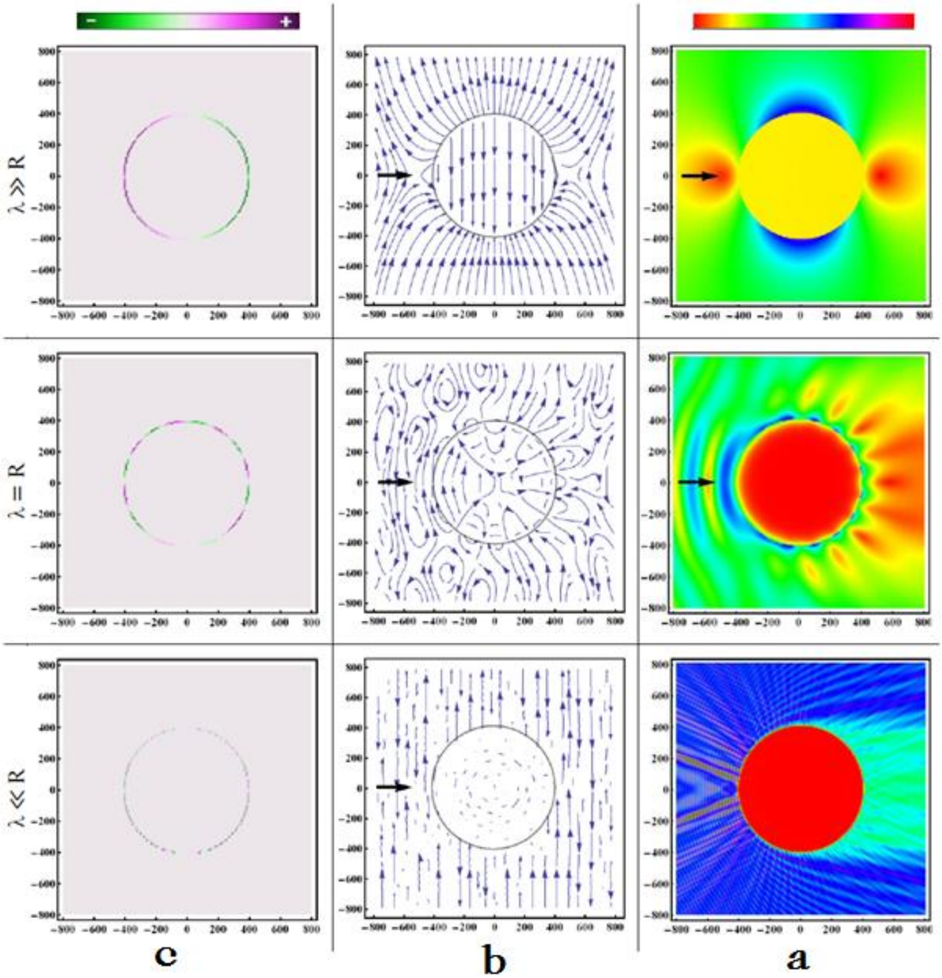

Fig. 4. Distribution of the field in and around,a plasmonic nanowires for λ>>R, λ = R and λ<<R. The electric field, (a)field lines, (b) and distribution of the charge density, (c). (axes are in nanometer).

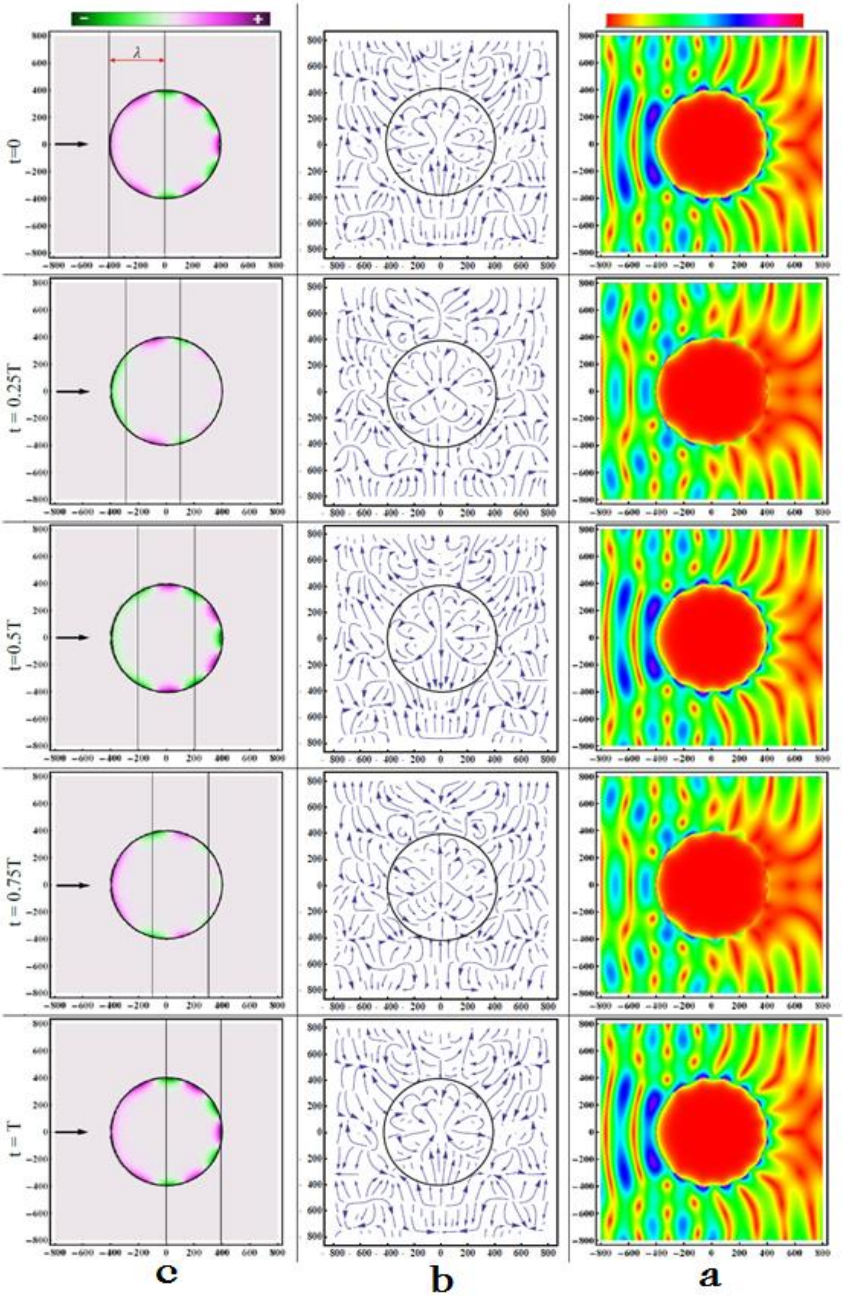

Fig. 5. Distribution of the field in and around a plasmonic nanowires for different times. The electric field, (a) field lines, (b) and distribution of the charge density, (c). (axes are in nanometer).

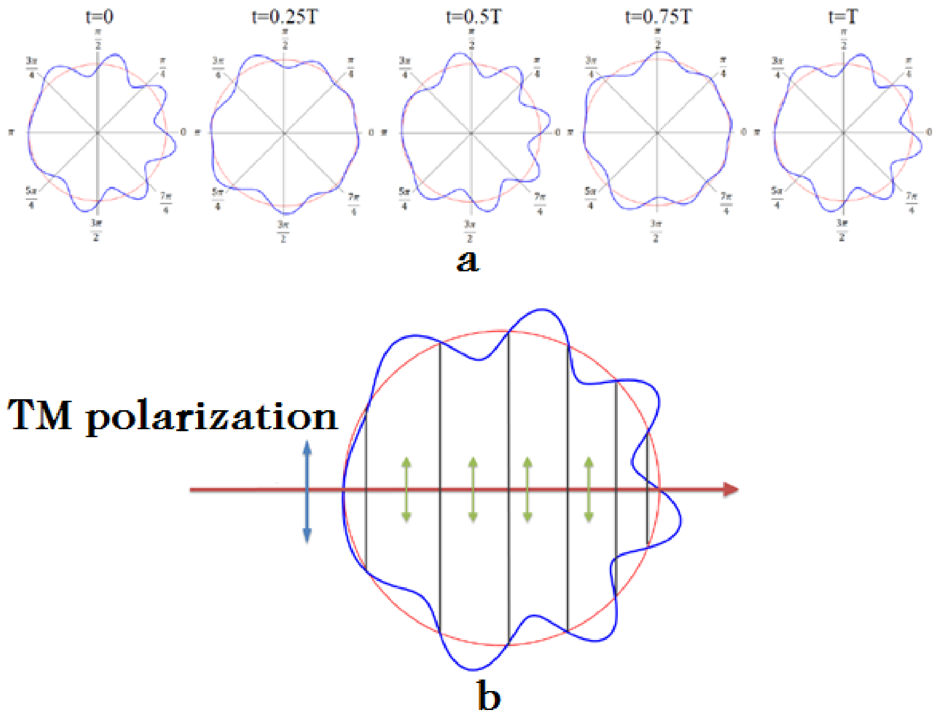

Fig. 6. Diagram of surface charge density on the boundary of nanowire. (a) For various times from 0 to T and (b) themmagnified diagram of time t = 0.

4. Conclusion

In this paper, the method of integral equations to simulate light scattering and study plasmonic effects was used. A nanowire with circular cross-section of radius 400 nm was considered in the simulations and various conclusions were obtained:

1- Simulation oflight scatteringof non-plasmonic nanowire like glassshowed thatno trace ofsurface Plasmon excitationis seen and only refractionoccurs. Simulation of TElight scattering from plasmonicnanowiresalso reveals formation of no surface plasmon. Simulationsshowed that in theTMlight scattering from plasmonicnanowires, surface Plasmon excitation is seen.

2- Simulation of TM light scattering from plasmonic nanowire withdifferent wavelengths indicated that for long wavelengths the electrostatic case is seen and localized surface plasmon is constructed with no trace of the geometric shadow or diffraction at the back side. For wavelengths that are comparable to the diameter of the nanowire simulations show the diffraction phenomenon. For small wavelengths, simple geometrical shadow is formed.

3- Simulation of temporal evolution of field and distribution of chargethroughTM light scattering from plasmonic nanowire showed that the surface field distribution moves in a wave-like motion.These resultscould be useful in calculating of velocity of surface palsmon waves which is our future work.

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