Enhanced Nonlinear Effect of Lithium Niobate Based Periodic Nano-antenna Array

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Abstract. We report nonlinear properties of lithium niobate based periodic nano-antenna array. The resonances of this nano-antenna array can be engineered by tuning the geometrical parameters. The nonlinear effect gets enhanced when the electric and magnetic resonances overlap.

1. Introduction

It is well known that nano-antenna can precisely control electromagnetic waves owing to its subwavelength structure. Research on nano-antenna has become a new focus because of its diverse applications, including thermal absorption [1-3] and biomedicine [4-6]. Furthermore, the strong field confined to a small region due to electromagnetic resonances in nano-antenna provides a new way to study nonlinear effects. However, conventional metallic nano-antenna manipulates electromagnetic field with their surface plasmon resonance which is difficult to tune, and it also manifests large ohmic losses. In addition, these metals, which are typically used to fabricate the nano-antenna, are also not ideal nonlinear materials. In this regard, dielectric nano-antenna adequately overcomes these drawbacks. Unlike metal, dielectric nano-antenna has low ohmic losses [7-9] and higher intrinsic nonlinearity. Particularly, lithium niobate is an important candidate for dielectric nano-antenna because of its multifunctional photoelectric and highly nonlinear characteristics specifically, second order nonlinear susceptibility.

In dielectric nano-antenna, electric and magnetic resonances occur when the incident light wavelength satisfies certain condition corresponding to the geometry of the nano-structure [10]. These resonances lead to strong electric field confinement in the nano-antenna [11,12]. In the lithium niobate based dielectric nano-antenna, different kind of electromagnetic resonances can be induced in different wavelength regime. The wavelength position of electric and magnetic resonances can be changed by manipulating the shape and size of the nano-antenna [13] as the resonance-wavelength is related to the geometry of the nano-antenna. The nonlinear effects can be further enhanced by strong electric field which can be achieved by overlapping the electric and magnetic resonances. This overlapping can be obtained by manipulating the shape and size of the nano-antenna structure [14].

2. Multipole

When electromagnetic wave is incident on a non-magnetic nanoparticle, polarization current will be generated. This polarization current can be derived using Poynting theorem when the surrounding medium is nonmagnetic ($\mu_r = \varepsilon_r = 1$). Total extinction power can be calculated following the equation given by [10]
\[ P_{\text{ext}} = \text{Im} \left( \frac{\rho}{2} \int_{V} \mathbf{E}_0 \cdot \mathbf{P}(r) dV \right), \]  

where \( P_{\text{ext}} \) is the total extinction power, \( \mathbf{E}_0 \) is the electric field of the incident electromagnetic wave, \( \mathbf{P}(r) \) refers to the position, and \( \mathbf{P}(r) \) is the polarization vector induced in the nanoparticle by the incident electromagnetic wave. \( \mathbf{P}(r) \) can be expressed as

\[ \mathbf{P}(r) = \int_{V} \mathbf{P}(r') \delta(r - r') dV'. \]

The extinction power can be approximated to be the scattering power as the absorption is negligible. The total extinction power \( (P_{\text{ext}}) \) can be given by

\[ P_{\text{ext}} = P_{\text{ext}}^p + P_{\text{ext}}^m + P_{\text{ext}}^q + P_{\text{ext}}^M, \]

where \( P_{\text{ext}}^p, P_{\text{ext}}^m, P_{\text{ext}}^q, \) and \( P_{\text{ext}}^M \) are electric dipole (ED), magnetic dipole (MD), electric quadrupole (EQ), and magnetic quadrupole (MQ), respectively. Only the first four electromagnetic multipole terms are considered as the higher order terms are negligible. \( P_{\text{ext}} \) can also be written as

\[ P_{\text{ext}} = \frac{c^2 k_0^2 Z_0}{12\pi} |\mathbf{p}|^2 + \frac{c^2 k_0^2 Z_0}{12\pi} |\mathbf{m}|^2 + \frac{1}{12\pi} |Q_{\alpha\beta}|^2 + \frac{1}{12\pi} |M_{\alpha\beta}|^2, \]

where

\[ \rho = \varepsilon_0 (1 - \varepsilon_r) \int_{V} E(r') dV', \]

\[ m = \frac{i \omega \varepsilon_0 (1 - \varepsilon_r)}{2\varepsilon} \int_{V} \mathbf{r} \times \dot{\mathbf{E}}(r') dV', \]

\[ Q_{\alpha\beta} = \frac{\varepsilon_0 (1 - \varepsilon_r)}{2} \int_{V} \left[ r_\alpha E_\beta + r_\beta E_\alpha - \frac{2}{3} (r \cdot \dot{\mathbf{E}}(r')) \delta_{\alpha\beta} \right] dV', \]

\[ M_{\alpha\beta} = \frac{i \omega \varepsilon_0 (1 - \varepsilon_r)}{3\varepsilon} \int_{V} \left[ (\mathbf{r} \times \dot{\mathbf{E}}(r'))_\alpha r_\beta + (\mathbf{r} \times \dot{\mathbf{E}}(r'))_\beta r_\alpha \right] dV', \]

\[ c \] is the speed of light in vacuum, \( k_0 \) is the wavenumber of incident light in vacuum, and \( Z_0 \) is the free-space impedance. \( \alpha' \) and \( \beta' \) refer to the two of the three coordinates (x, y, z). The electromagnetic resonances, which are calculated using equation (4), are tuned by varying the size and shape of the nano-antenna.

3. Simulation

3.1. Structure of the nano-antenna

In order to analyse the characteristics of the lithium niobate based periodic nano-antenna array, following simulations are done. The inverted-cone antenna was modelled by the finite-difference time-domain method (FDTD Solutions). The schematic of the nano-antenna structure is shown in figure 1. In this case, both substrate and the nano-antenna are lithium niobate. Thus, we can fabricate the structure directly on the lithium niobate bulk which reduce the complexity of the process. The xz- or yz- cross-section of each unit is a trapezoid. The radius of the top surface is larger than that of the bottom surface for each unit. The slope, \( \theta \), of the side wall is about 80 degree. The simulation shows that the overlapping will be better if the structure has higher slope, but the difficulty of the fabrication increases sharply as the slope is increased. The periodicity of the nano-antenna array is \( T = 2 \times r_{\text{top}} \pm 200 \text{ nm} \), where \( r_{\text{top}} \) is the radius of the top surface. The whole system are illuminated by plane-wave with the \( -z \) direction. The boundary conditions of the \( z \) direction is perfectly matched layers. The mesh size used for the simulation was 10 nm.
3.2. Results and discussion

Figure 2 (a) shows the transmission spectrum of the periodic nano-antenna array. The radius of the top and bottom surfaces are 320 nm and 250 nm, respectively. The height of the nano-antenna is 430 nm. In the transmission spectrum (figure 2 (b)), the three marked valleys from right to left correspond to magnetic dipole, electric dipole, and magnetic quadrupole resonances, respectively. The magnetic quadrupole mode is mixed with the higher order modes and could not be identified in the transmission spectrum.

![Figure 1. Schematic diagram of nano-antenna array.](image)

**Figure 2.** (a) Simulated transmission spectrum of the periodic nano-antenna array. (b) 2D electric field distribution patterns corresponding to the three modes: magnetic dipole (MD), electric dipole (ED), and magnetic quadrupole (MQ) resonance.

For the simulations of nonlinear effects, the incident laser beam wavelength is chosen according to the resonant wavelength obtained from the transmission spectrum of the nano-antenna array. The second order nonlinear susceptibility of lithium niobate is $3 \times 10^{-11} \text{ m/V}^2$. From the simulation, we get the power of the second harmonic generation (SHG) (see figure 4 (a)).

Furthermore, the electric dipole and magnetic quadrupole resonances can be overlapped by varying the geometrical parameters of the nano-antenna (figure 3). Thereafter, we derive the SHG signal strength again (figure 4 (b)) and compare it with previous results. It demonstrates that the nonlinear effect gets enhanced when the two resonances are overlapped.
Figure 3. (a) Simulated transmission spectrum of the periodic nano-antenna array with $r_{\text{top}} = 240 \, \text{nm}$, $r_{\text{bottom}} = 170 \, \text{nm}$, $H=30 \, \text{nm}$, and $\theta = 80^\circ$.

Figure 4. Simulated transmission spectrum showing the peak corresponding to SHG with $r_{\text{bottom}} = 250 \, \text{nm}$ (a) and $170 \, \text{nm}$ (b).

4. Conclusion
We report nonlinear properties of lithium niobate based periodic nano-antenna array. The resonances of this nano-antenna array can be engineered by tuning the geometrical parameters. The electric field confined to the nano-antenna gets enhanced when resonance occur. Intensity of the field gets further enhanced if two of the resonances are overlapped. Therefore, the nonlinear effect can be enhanced by tuning the geometrical parameters of the nano-antenna.

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6. Reference
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