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Numerical analysis of second harmonic generation for THz-wave in a photonic crystal waveguide using a nonlinear FDTD algorithm

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ABSTRACT

We have presented a numerical analysis to describe the behavior of a second harmonic generation (SHG) in THz regime by taking into account for both linear and nonlinear optical susceptibility. We employed a nonlinear finite-difference-time-domain (nonlinear FDTD) method to simulate SHG output characteristics in THz photonic crystal waveguide based on semi insulating gallium phosphide crystal. Unique phase matching conditions originated from photonic band dispersions with low group velocity are appeared, resulting in SHG output characteristics. This numerical study provides spectral information of SHG output in THz PC waveguide. THz PC waveguides is one of the active nonlinear optical devices in THz regime, and nonlinear FDTD method is a powerful tool to design photonic nonlinear THz devices.

1. Introduction

Significant progress of terahertz (THz) technologies have been seen to study wide scientific fields such as material science, life science, chemistry, high-speed communication, and non-destructive inspection [1,2]. However, the pulse energies produced by THz sources were limited in comparison with the optical frequency region. Recently, intense THz wave sources have been developed, which leads to the realization of nonlinear THz experiments which have been a considerable interest. These THz sources are based on pulse front tilted optical rectification [3], optical mixing in a laser generated plasma [4], and THz parametric generation [5]. To extend THz experiments into the nonlinear regime, effective nonlinear optical (NLO) interactions in the NLO devices is essential. One of the promising devices is photonic crystal (PC) structure.

PCs have been widely studied in the optical region owing to unique optical characteristics such as slow light propagation and existence of photonic band gap, and show a strong confinement of light [6–8]. Variety of applications by utilizing linear and nonlinear optical properties of PCs have been developed such as, waveguides, cavities, lasers, optical switches and nonlinear optical mixing [9–12]. In the THz frequency regime, the considerable progress of THz PC component has been made by the development of linear and THz photonic devices [13–15]. Nonlinear PC devices are of great interest because the strong confinement and Bloch wave characteristics appear in PC structures. These features lead to the unique phase-matching condition for THz wave [16–18].

The advent of fast and powerful computers has made detailed numerical modeling an efficient and reliable tool for researchers and engineers. Since the introduction of the Yee algorithm for the numerical solution of Maxwell's equations in 1966 [19], the finite-difference-time-domain (FDTD) method has been applied to the simulation of a large number of nonlinear as well as linear problems. Recently, a nonlinear FDTD method by modifying Yee's algorism has been developed as a powerful simulation tool to describe nonlinear phenomena such as second or third harmonic generation, THz wave generation via optical rectifications in the PhC structures where phase matching is obtained by engineering the dispersion of the Bloch modes [20–23].

In this paper, we formulate the full-wave model for second harmonic generation (SHG) in optical structure containing second order nonlinearity. We conduct the numerical simulation of the second harmonic generation in the THz PC waveguide via the vectorial nonlinear (NL)-FDTD. We employed this method to simulate the SHG process in gallium phosphide (GaP) based PC waveguide. Our numerical results provide the THz-wave output spectra based on the PC waveguide guiding modes.

2. Theoretical modeling for nonlinear FDTD

We start by the formulation of the SHG process ($\omega_s = 2\omega_f$) in nonlinear (NL)-FDTD method. This method is based on a modification of the original Yee's FDTD algorithm. The original FDTD

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solves the coupled linear Maxwell's equations in the differential form, written as

$$\frac{\partial H}{\partial t} = -\frac{1}{\mu_0}\nabla \times E, \tag{1}$$

$$\frac{\partial E}{\partial t} = -\frac{1}{\varepsilon_r}\nabla \times H - \frac{1}{\varepsilon_r}\frac{\partial P^{\mathrm{NL}}}{\partial t}, \tag{2}$$

where E and H are the electric and magnetic field intensity. μ_0, P^{NL} are magnetic permeability and nonlinear polarization created by the incident pump wave. Here, we took into account for the Lorentz dispersion of GaP in the THz region during the calculation of the NL-FDTD. Permittivity ε_r of GaP in the THz region is expressed by Lorentz dispersion relation [24],

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{2\omega_{\mathrm{TO}}^2}{\omega_{\mathrm{TO}}^2 - \omega^2 + i\omega\gamma_{\mathrm{TO}}}, \tag{3}$$

where ε_∞ $(= 9.2)$, ω_p and γ_d are static dielectric constant, plasma frequency and its damping constant, and $\omega_{\mathrm{TO}}/2\pi$ $(=11.01$ THz) and $\gamma_{\ \mathrm{TO}}(=0.03$ THz) are transverse optical phonon frequency and phonon damping constant. Here, we consider a semi-insulating GaP crystal as a NLO material which possesses low carrier density below 10^{12} cm^{-3}. Therefore, the contribution of free carrier to the linear dispersion relationship can be ignored.

The second-order nonlinear susceptibility tensor $\chi^{(2)}_{\mathrm{SHG}}$ below the TO phonon resonance frequency ω_{TO} displays strong dispersion relation as well as linear dispersion relation. The dispersion of $\chi^{(2)}_{\mathrm{SHG}}$ below the phonon resonances is given by the following expression [25]:

$$\chi^{(2)}_{\mathrm{SHG}}(2\omega;\ \omega,\ \omega) = \chi^{(2)}_{\infty}\Delta(\omega,\ \omega), \tag{4}$$

where $\chi^{(2)}_{\infty}(=134$ pm/V [25]) is the nonlinear susceptibility that depends on the purely electronic response,

$$\Delta(\omega,\ \omega) = 1 + C_1\left(\frac{2}{D(\omega)} + \frac{1}{D(2\omega)}\right) + C_2\left(\frac{2}{D(\omega)^2} + \frac{2}{D(\omega)D(2\omega)}\right) + C_3\left(\frac{1}{D(\omega)^2 D(2\omega)}\right), \tag{5}$$

where $D(\omega) = 1 - \omega^2/\omega_{\mathrm{TO}}^2 - i\gamma_{\mathrm{TO}}\omega/\omega_{\mathrm{TO}}^2$ is the resonance denominator with phonon damping. C_1, C_2, and C_3 are dimension less coefficients whose values are -0.27, -0.04, and -0.53, respectively. Fig. 2 displays the dispersion relations of linear and nonlinear susceptibilities as described by Eqs. (3), (4) and (5). These dispersion relations show monotonous increment as THz frequency increase monotone, respectively. In the NFDTD simulation, we take into account for the dispersive characteristics of the nonlinear material of GaP.

One of the approaches to treat the dispersive medium in the NL-FDTD algorithm is known as the recursive convolution (RC) method [26]. In a linear and nonlinear dispersive medium, the electric flux density and nonlinear polarization intensity are related to the electric field intensity by

$$\boldsymbol{D}(t) = \varepsilon_0\varepsilon_\infty\boldsymbol{E}(t) + \varepsilon_0\int_0^t \boldsymbol{E}(t-\tau)\chi(\tau)d\tau, \tag{6}$$

$$\boldsymbol{P}^{\mathrm{NL}}(t) = \varepsilon_0\int_0^t (\boldsymbol{E}(t-\tau))^2\chi^{(2)}_{\mathrm{SHG}}(\tau)d\tau, \tag{7}$$

where ε_0 is the permittivity of free space, ε_∞ is the dielectric constant of the medium at infinite frequency, and $\chi(t)$ is a linear susceptibility function of the NLO medium in the time domain associated with the dielectric function expressed in Eq. (3).

In the NL-FDTD simulation with the RC method, we estimate the convolution integral by approximating the electric field to be constant during the time interval Δt.

In the vectorial form, the nonlinear polarization for the fundamental and the second harmonic waves are expressed by [27]

$$\begin{bmatrix} P_X^{NL,f} \\ P_Y^{NL,f} \\ P_Z^{NL,f} \end{bmatrix} = \varepsilon_0\boldsymbol{\chi}^{(2)}_{\mathrm{SHG}}(2\omega;\ \omega,\ \omega)\begin{bmatrix} E_X^f E_X^s \\ E_Y^f E_Y^s \\ E_Z^f E_Z^s \\ E_Z^f E_Y^s + E_Y^f E_Z^s \\ E_Z^f E_X^s + E_X^f E_Z^s \\ E_X^f E_Y^s + E_Y^f E_X^s \end{bmatrix}, \tag{8}$$

$$\begin{bmatrix} P_X^{NL,s} \\ P_Y^{NL,s} \\ P_Z^{NL,s} \end{bmatrix} = \frac{1}{2}\varepsilon_0\boldsymbol{\chi}^{(2)}_{\mathrm{SHG}}(2\omega;\ \omega,\ \omega)\begin{bmatrix} E_X^f E_X^f \\ E_Y^f E_Y^f \\ E_Z^f E_Z^f \\ 2E_Y^f E_Z^f \\ 2E_X^f E_Z^f \\ 2E_X^f E_Y^f \end{bmatrix} \tag{9}$$

where P_l^{NL} $(l=X,\ Y,\ Z)$ is the nonlinear polarization component indicated by the crystallographic coordinate along [100], [010], and [001] directions, respectively. The optical coefficient tensor of GaP is given by:

$$\frac{1}{2}\left|\chi^{(2)}_{\mathrm{SHG}}(2\omega;\ \omega,\ \omega)\right| = d(2\omega;\ \omega,\ \omega) = \begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{bmatrix} \tag{10}$$

In this case, coupling of TM-like fundamental mode of THz wave to TE-like second harmonic mode is possible, resulting differential equations for TM-like fundamental input are:

$$\varepsilon_r\frac{\partial E_X^f}{\partial t} = -\frac{\partial H_Y^f}{\partial Z} - 2\varepsilon_0 d_{14}\frac{\partial P_X^{NL,f}}{\partial t}, \tag{11}$$

$$\varepsilon_r\frac{\partial E_Y^f}{\partial t} = -\frac{\partial H_Z^f}{\partial X} - 2\varepsilon_0 d_{14}\frac{\partial P_Y^{NL,f}}{\partial t}, \tag{12}$$

$$\mu_0\frac{\partial H_Z^f}{\partial t} = \frac{\partial E_X^f}{\partial Y}. \tag{13}$$

Those for TE-like second harmonic output are:

$$\varepsilon_r\frac{\partial E_Y^s}{\partial t} = \left(\frac{\partial H_Z^s}{\partial X} - \frac{\partial H_X^s}{\partial Z}\right) - 2\varepsilon_0 d_{14}\frac{\partial P_Y^{NL,s}}{\partial t}, \tag{14}$$

$$\mu_0\frac{\partial H_X^s}{\partial t} = \frac{\partial E_Y^s}{\partial Z}, \tag{15}$$

$$\mu_0\frac{\partial H_Z^s}{\partial t} = -\frac{\partial E_Y^s}{\partial X}. \tag{16}$$

Here, we consider the THz wave propagation with frequency $\omega_{\mathrm{THz}}/2\pi$ and $2\omega_{\mathrm{THz}}/2\pi$ in this simulation to describe the SHG process. By discretizing the simulation domain into a finite computational grid, the magnetic and electric fields are computed at interlacing time intervals, as shown here for the fundamental $E_X{}^{\mathrm{f}}$ component: