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Second harmonic generation in photonic crystals: numerical simulation

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In this paper, we want to present a simple and efficient numerical method for SHG analysis in one-dimensional photonic crystals (PhCs) based on full nonlinear system of equations. For solving the nonlinear SHG problem we used a simple method of finite elements coupled with fixed point iteration. Our model does not need additional analytic approximation compared with some existing methods, and it can be easily extended to study the SHG problem in two-dimensional photonic crystals. We used the FlexPDE Professional program to plot the diagrams varying the parameters. At the end we obtained two maximum intensities of the second harmonic wave within each high index layer, that being in contrast to the fundamental wave peak. This result can be found also in the literature. In addition, we have plotted the lattice using the Optiwave FDTD software and we observed the propagation of the field in time.

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1. Introduction

Photonic crystals are periodic structures with the periodicity proportional to the wavelength of the electromagnetic wave (Fig. 1.1), having a forbidden band which blocks the propagation of light in a specific frequency range [1-4]. This property allows control over light effects that would otherwise be very difficult to control with conventional optics [5-8].

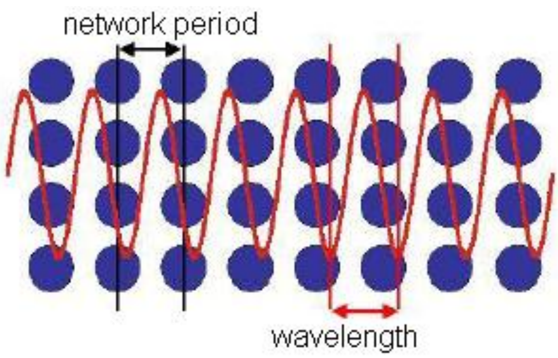

Fig. 1. The path of an electromagnetic wave in a periodic structure with the network constant "a".

In recent years, progress in photonic technology has generated a trend toward integration of electronic and photonic devices. The latter offer several advantages over the former: high working speed, size, good reliability.

A class of photonic materials that were created theoretically and experimentally in 1991 by E. Yablonovitch are materials with "photonic band gap" (PBG), which are known as "photonic crystals"[1,13].

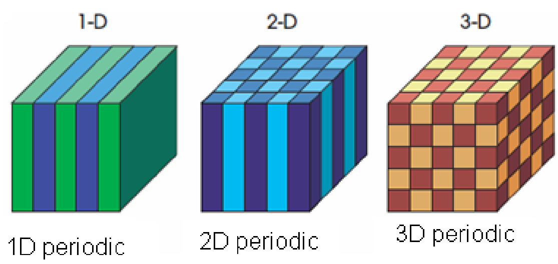

Fig. 2. Examples of 1D,2D,3D PhCs. Different colors represent materials with different dielectric constant.

In the last few years, nonlinear optical processes such as second harmonic generation (SHG) in nonlinear photonic crystals have attracted a great interest. Nonlinear photonic crystals offer unique and fundamental methods of enhancing various nonlinear optical processes [9-12].

We used nonlinear Helmholtz equations [2-4], which are based on Maxwell's equations. The nonlinear problem has a unique solution only if the importance of the nonlinear susceptibility tensor is not too large.

We solved the scalar nonlinear Helmholtz system using a combination of finite elements method and fixed point iterations. To find the solutions of nonlinear equations we replaced the unknown functions repeatedly from the right side with the previous approximations.

This model does not require any additional analytical approximations and it can be easily extended to two-dimensional structures of photonic crystals.

There are two ways to improve the second harmonic generation in nonlinear photonic crystals. The first one is to adjust simultaneously the fundamental wave frequencies and the second harmonic wave (SHW) to the localized frequencies at the photonic band edge. The second one is to introduce defects coming from the nonlinear materials in photonic crystals.

Using the first method, the density of the electromagnetic fields increases, and phase superposing can occur. Thus, the second harmonic generation will be improved. In the second method, we improve the generation of the second harmonic using strong localized fields in the defect area.

2. Nonlinear problem

We consider a nonlinear material with N layers. The structure is considered periodic along the z direction, for $0 \le z \le D$, and the media is considered to be non-magnetic with a constant magnetic permittivity. Considering that the fundamental frequency and the SHW are given in the transverse electric polarization (TE), the equations for SHG are:

$$\frac{d^2E_1}{dz^2} + (k_0 n_1)^2 E_1 = -k_0^2 \chi_1^{(2)} \bar{E}_1 E_2 \quad (1)$$

$$\frac{d^2E_2}{dz^2} + (2k_0 n_2)^2 E_2 = -2k_0^2 \chi_2^{(2)} E_1^2 \quad (2)$$

where E_1 and E_2 are the electric fields for the fundamental frequency (FF) x and for the SH frequency $2x$. $\bar{E}_1$ is the complex conjugate, $k_0 = \omega/c$ is the wave number in vacuum, c is the speed of light in vacuum, n_1 and n_2 are the refractive indices of ω and 2 ω, and $\chi_1^{(2)}$ and $\chi_2^{(2)}$ are two second order elements of the nonlinear susceptibility tensors for ω and 2 ω.

We assume that the structure is linear for $z < 0$ and $z > D$. The nonlinear structure of the PhC is situated between two linear materials with refractive index n_a $(z < 0)$ and n_b $(z > D)$.

When the incident light is normal on the sample surface along the z direction we have:

a) region $z < 0$

$$E_1(z) = E_i \exp(-i\alpha_a z) + E_{1r} \exp(i\alpha_a z)$$

$$E_2(z) = E_{2r} \exp(i\beta_a z),$$

where the incident electric field is $(0, E_i \exp(-i\alpha_a z), 0)$and $\alpha_a = k_0 n_a$, $\beta_a = 2k_0 n_a$,$E_{1r}$and $E_{2r}$are reflectivity constants for ω and 2 ω frequencies.

b) region $z > D$

$$E_1(z) = E_{2t} \exp(-i\alpha_b z)$$

$$E_2(z) = E_{2t} \exp(-i\beta_b z)$$

where $\alpha_b = k_0 n_b$, $\beta_b = 2k_0 n_b$,E_{1t} and E_{2t} are transmittance constants for ω and 2 ω frequencies.

The tangential components of E and H must be continuous at the boundary, which define the interface between the two homogeneous materials, and the normal components of D and H must be continuous at the boundary for all frequencies. Because the tangential components of E_j and H_j are continuous for $z = 0$ and $z = D$, we obtain the following boundary conditions for the first and the last point:

$$E_1(0) = E_i + E_{1r} \quad (3)$$

$$E_2(0) = E_{2r} \quad (4)$$

$$E_1(D) = E_{1t} \exp(-i\alpha_b D) \quad (5)$$

$$E_2(D) = E_{2t} \exp(-i\beta_b D) \quad (6)$$

$$\frac{dE_1}{dz}(0) = -i\alpha_a E_i + i\alpha_a E_{1r} \quad (7)$$

$$\frac{dE_2}{dz}(0) = i\beta_a E_{2r} \quad (8)$$

$$\frac{dE_1}{dz}(D) = -i\alpha_b E_{1t} \exp(-i\alpha_b D) \quad (9)$$

$$\frac{dE_2}{dz}(D) = -i\beta_b E_{2t} \exp(-i\beta_b D) \quad (10)$$

From (3) to (10) we obtain:

$$\frac{dE_1}{dz}(0) = -2i\alpha_a E_i + i\alpha_a E_i(0) \quad (11)$$

$$\frac{dE_2}{dz}(0) = i\beta_a E_2(0) \quad (12)$$

$$\frac{dE_1}{dz}(D) = -i\alpha_b E_i(D) \quad (13)$$

$$\frac{dE_2}{dz}(D) = -i\beta_b E_2(D) \quad (14)$$

We define the domain $\Gamma = (0, D)$. We must solve the coupled nonlinear Helmholtz equations (1) and (2) in Γ, using the previous boundary conditions (12) - (14).

3. Numerical method

We solve the nonlinear problem with a combination between the finite elements method and fixed point iterations. We consider a test function ψ. The variational problem corresponding to our nonlinear equations could come from the classical variational technique.

We first multiply both sides of equations (2.1) and (2.2) with $\bar{\psi}$, then we integrate on the domain Γ. The result is:

$$\int_\Gamma \left(\frac{d^2E_1}{dz^2} + k_0^2 n_1^2 E_1 \right) \bar{\psi} ds = \int_\Gamma -k_0^2 \chi_1^{(2)} \bar{E}_1 E_2 \bar{\psi} ds$$
$$\int_\Gamma \left(\frac{d^2E_2}{dz^2} + 4k_0^2 n_2^2 E_2 \right) \bar{\psi} ds = \int_\Gamma -2k_0^2 \chi_2^{(2)} E_1^2 \bar{\psi} ds$$

where $\bar{\psi}$ is the complex conjugate of ψ. Since the usual boundary conditions at the interface between two homogeneous materials are valid we have:

$$[E_j]_{z_n} = 0,\ \left[\frac{dE_j}{dz}\right]_{z_n} = 0,\ j = 1,2,\ldots$$

where $[*]_{z_n}$ is the "jump" at the interface $z = z_n$. We use integration by parts and the boundary conditions (2.12) - (2.14), and we obtain the following variational relation:

$$a(E_1,\psi) + i\alpha_a E_1(0)\bar{\psi}(0) + i\alpha_b E_1(D)\bar{\psi}(D) = 2i\alpha_a E_i \bar{\psi}(0) + k_0^2 \int_\Gamma \chi_1^{(2)} \bar{E}_1 E_2 \bar{\psi} ds \quad (15)$$

$$b(E_2,\psi) + i\beta_a E_2(0)\bar{\psi}(0) + i\beta_b E_2(D)\bar{\psi}(D) = 2k_0^2 \int_\Gamma \chi_2^{(2)} E_1^2 \bar{\psi} ds \quad (16)$$

where:

$$a(E_1,\psi) = \int_\Gamma \left(\frac{dE_1}{dz}\frac{d\bar{\psi}}{dz} - k_0^2 n_1^2 E_1 \bar{\psi} \right) ds$$
$$b(E_2,\psi) = \int_\Gamma \left(\frac{dE_2}{dz}\frac{d\bar{\psi}}{dz} - 4k_0^2 n_2^2 E_2 \bar{\psi} \right) ds$$

The solution of equations (1) and (2) taking into consideration the boundary conditions (12) - (14) gives the solution for the variational problem (15) and (16).

For a given E_i the variational problem has a unique solution E_1, E_2 when the product between $\left\| k_0^2 \chi_1^{(2)} \right\|_{L^\infty}$ and $\left\| 2k_0^2 \chi_2^{(2)} \right\|_{L^\infty}$ is not too high. The nonlinear variational problem (15) and (6) is well determined too, and we can calculate the unique solution of the SHG problem in the nonlinear 1D PhC structures.

Our problem can be solved by repetitive replacement of $E_1\ and\ E_2$ with the previous approximations on the right side, using the solution from (15).

The numerical diagram is divided into the following steps:

Step 1: Use the finite elements method to find $E_{1,0}$, when $E_{1,0}$ satisfies:

$$a(E_{1,0},\psi) + i\alpha_a E_{1,0}(0)\bar{\psi}(0) + i\alpha_b E_{1,0}(D)\bar{\psi}(D) = 2i\alpha_a E_i \bar{\psi}(0)$$

Step 2: Use the finite elements method to find $E_{2,0}$, when $E_{2,0}$ satisfies:

$$b(E_{2,0},\psi) + i\beta_a E_{2,0}(0)\bar{\psi}(0) + i\beta_b E_{2,0}(D)\bar{\psi}(D) = 2k_0^2 \int_\Gamma \chi_2^{(2)} E_{1,0}^2 \bar{\psi} ds$$

Step 3: For $k = 0, 1, 2, \ldots$, find $E_{1,k+1}$ and $E_{2,k+1}$ when resolving the variational problem (15) and (16) with $E_j = E_{j,k}$ on the right side.

Our numerical method combines the fixed point iterations for the nonlinear problem and the finite elements method for each variational equation.

The iteration scheme is no longer valid when the intensity of the incident electric field or the product between $\left\| k_0^2 \chi_1^{(2)} \right\|_{L^\infty}$ and $\left\| 2k_0^2 \chi_2^{(2)} \right\|_{L^\infty}$ is very high. It is well known that the majority of nonlinear optical materials have a very low nonlinear susceptibility. For all conventional materials the convergence of our method is rapid [5-10].

4. Numerical results

Numerically, we tested our method on a simple structure made of a nonlinear material with N layers, surrounded by vacuum. It is a one-dimensional system composed of 40 dielectric layers and the refractive index alternates between a high and a low value, $n_1^N = 1.42857$ and $n_1^L = 1.0$. For a reference wavelength $\lambda_0 = 1.0\mu m$, layers are $d_L = \lambda_0/(4n_1^L)$ and $d_N = \lambda_0/(2n_1^N)$ thick. Since the background medium is vacuum, we have $n_0 = n_b = 1.0$.

The efficiency of SHG conversion in nonlinear PhC can grow, while we simultaneously adjust the frequencies of the fundamental wave (FW) and of the SHW for the localized frequencies at the edge of photonic band. Thus, we investigate the generation of the SHW near the low frequency from the photonic band edge: Ω≈0.6.

We fix $n_2^N = 1.519$ and $n_2^L = 1.0$ and we take a small value for the nonlinear susceptibility tensor $\chi^{(2),N} = 0.1pm/V$. We assume that nonlinearity is uniformly distributed on the PBG structure. We calculate the SH field for a number of frequencies when the incidence wave is $E_i = 1.0 \times 10^6 V/m$.

The absolute value of the SHW at $z=D$ versus Ω for the FF is shown in Fig. 3. The huge amplification of SHG occurs when the frequency of an incident wave at a low frequency is carried away at the end of the band and it has a maximum value for Ω=0.592.

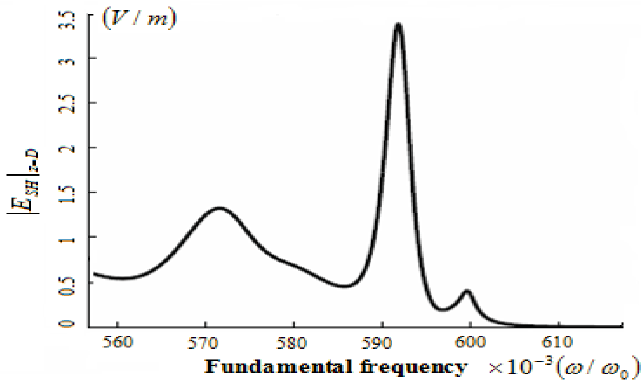

Fig. 3. The absolute value of SHG wave at z=D versus Ω.

In fig. 4 we represented the absolute value of the FF field and SH field for Ω=0.592. The FF is increased with more than one order of magnitude compared to the peak value outside the structure. So, the conversion efficiency of SHG should increase significantly. Because of the wavelength of the SH signal, which is half of the pumped wave, there are two maximum intensities of the SH wave within each high index layer (in contrast to the FW peak).

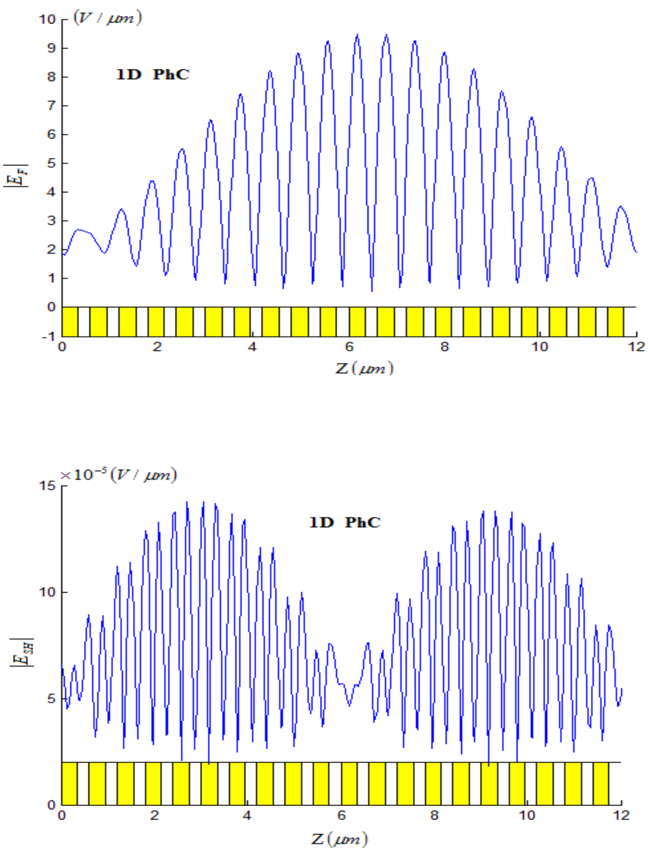

Fig. 4. The absolute value of the FF field and the SH field: the first one is the FW and second one is the SHW.

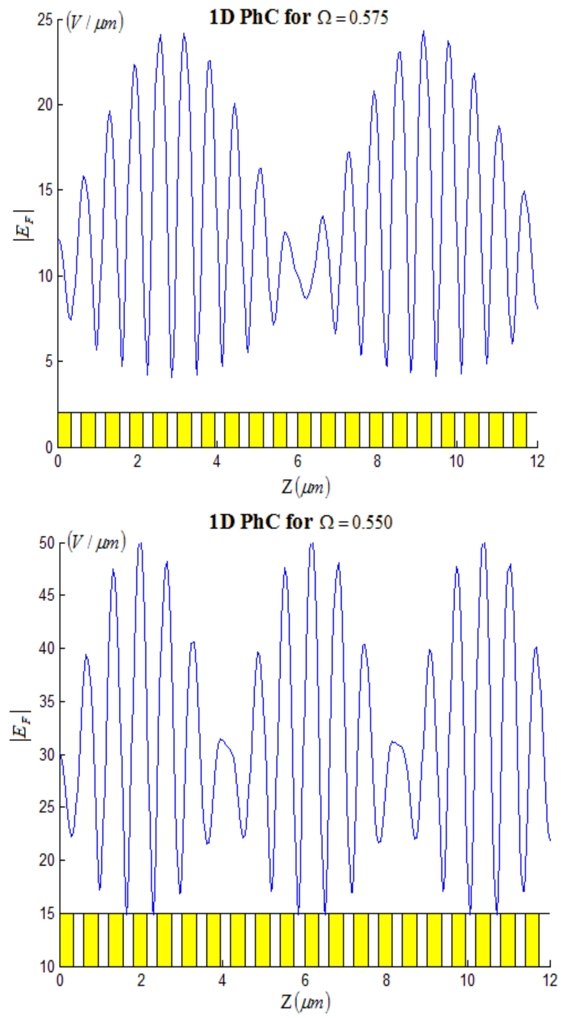

Fig. 5. The absolute value of the SH field: the first one is the fundamental wave at Ω=0.575 and the second one is the fundamental wave at Ω=0.550.

The Optiwave FDTD Software has three basic components:

- OptiFDTD_Profile Designer, where the materials used in the simulations are defined.
- OptiFDTD_Designer, where crystal structures are constructed, based on the materials defined in the Profile Designer.
- OptiFDTD_Analyzer, where the results obtained in the simulations are studied.

We have designed with OptiFDTD Designer a 1D photonic crystal structure using air as basic element (ε_1=1) and a photonic band gap cell lattice with ε_2=2.0408. The materials were previously defined in the Profile Desiger. The lattice constant is a=0.6μm and layers are $d_N = 0.35\mu m$ and $d_L = 0.25\mu m$ thick.

The results returned by Opti_FDTD Analyzer showed that the wave goes from entrance to exit with 25.04% losses. Losses of the beam energy are determined by absorption in the material and various nonlinear effects.

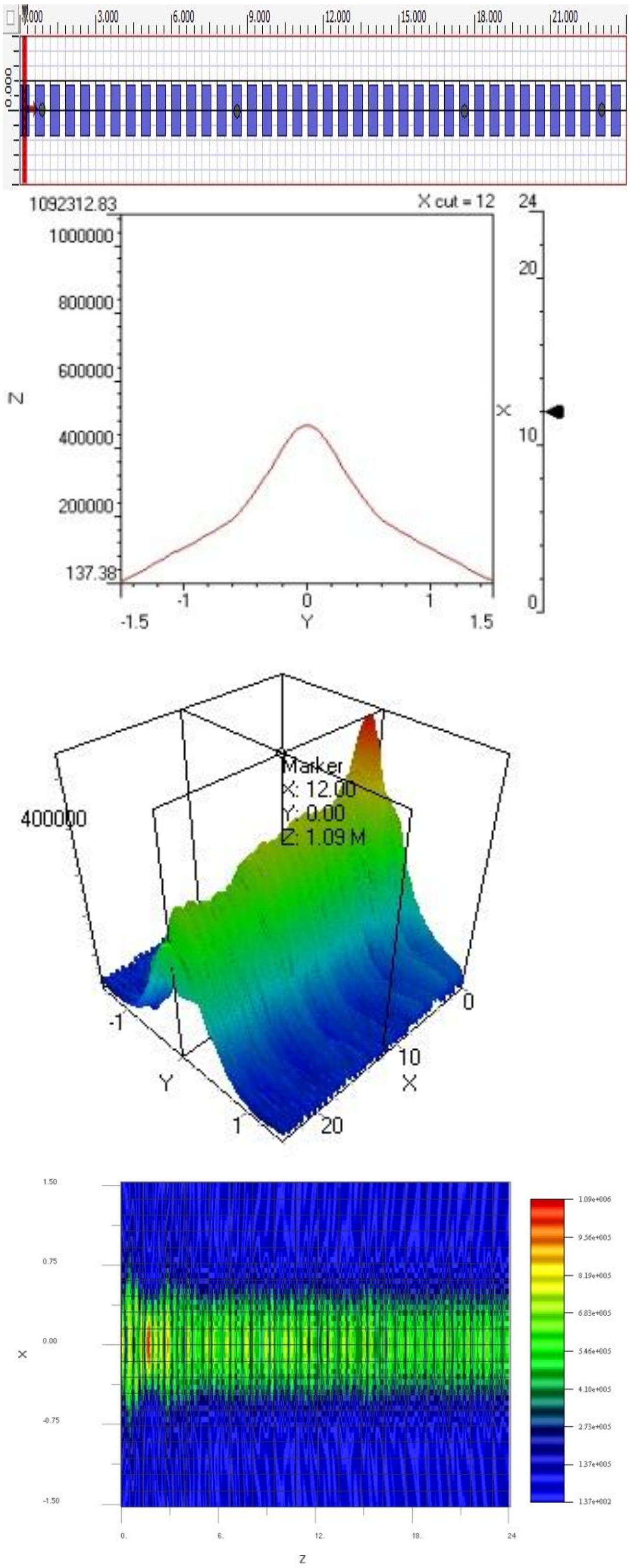

Fig. 6. The 1D photonic crystal lattice and field maps

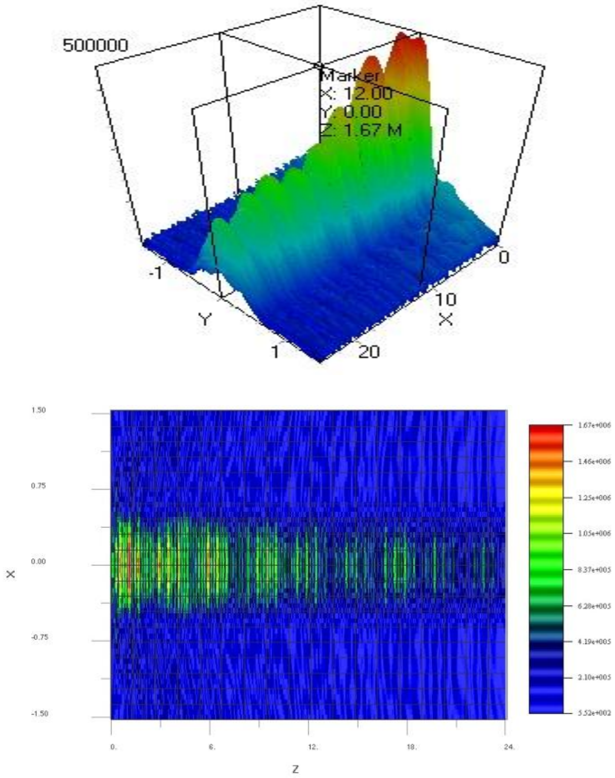

Fig. 7. Field maps for SH.

The second example is a PhC with defect. The perfect PhC is designed to be composed of standard materials N layers. We chose $LiNbO_3$ and air with nonlinear, respectively linear layers. The parameters of the 1D PhC structure are the following: the thickness and refractive indices of linear and nonlinear layers are $d_L = 0.351\mu m$, $d_N = 0.304\mu m$, $n_1^N = 2.157$, $n_1^L = 1.0$.

The second order nonlinear coefficient of the $LiNbO_3$ layers is assumed to be $\chi^{(2),N} = 87.8pm/V$ and the refractive index of $LiNbO_3$ for the SH frequency is $n_2^N = 2.237$. The incident wave is $E_i = 0.5 \times 10^6 V/m$. If the perfect structure is affected in any way the result of any permitted states at PBG may produce a rise of the field in the defect. Because of the nonlinearity of the material, SHG can grow significantly. We introduce a defect by changing the central layer thickness (the 15th layer of a total of 29 layers) from 0.304 to 0.737μm. We study the generation of the SHW around the fundamental wavelength $\lambda_{FW} = 1.064\mu m$.

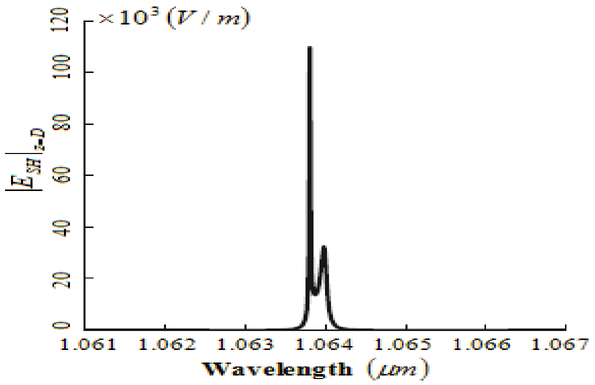

Fig. 8 The absolute value of SHW generation for a photonic crystal with defect at z=D .

The absolute value of the FF and the SH fields at the fundamental wavelength $\lambda_{FW} = 1.064\mu m$ in this structure with a defect is shown in Fig. 9.

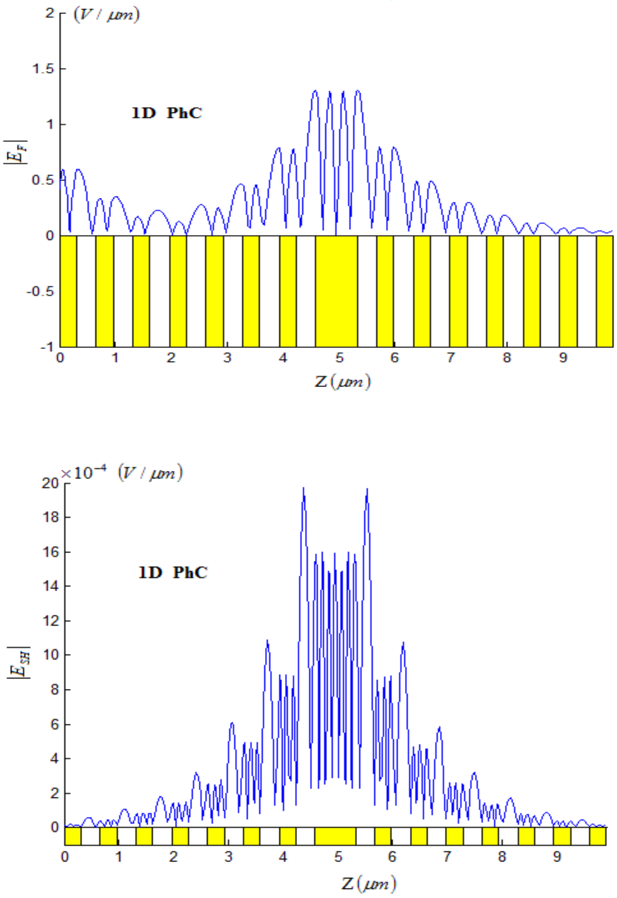

Fig. 9. The absolute value of FF field and of the SH field for the example with defect: the first one is the FW and the second one is the SH wave.

The fundamental frequency field and the second harmonic field from the defect grow simultaneously.

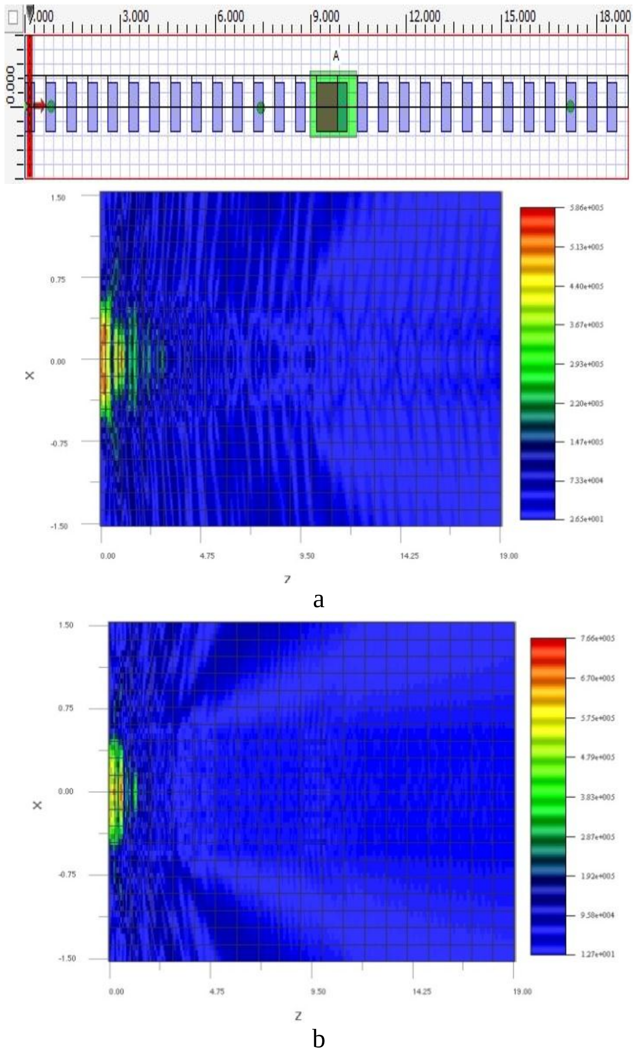

Fig. 10. The 1D photonic crystal lattice with defect on the 15th cell and field maps for FW (a) and for SH (b)

5. Conclusions

As a conclusion to fig. 5 we can add that we are dealing with a resonant character of the transfer characteristic of the photonic crystal. It allows to pass a frequency band, but the quality factor is different. This is explained by the dependence of the amplitude by the frequency.

We have presented a simple and efficient numerical method for the analysis of SHG in one-dimensional photonic crystals based on the fully nonlinear equations. The entire SHG nonlinear problem is solved by a simple a combination of finite elements method and fixed point iterations. In contrast with other methods our model does not require additional analytical approximations and it is easily extended for studying the problem of SHG in two-dimensional photonic crystals.

Because the nonlinear optical materials have very low nonlinear susceptibility, our method converges rapidly. Generally, less than ten repetitive steps are sufficient.

We used the FlexPDE Professional program to plot the diagrams varying the parameters. At the end we obtained two maximum intensities of the second harmonic wave within each high index layer, that being in contrast to the fundamental wave peak. This result is also found in the literature.

In addition, we build a 1D photonic crystal lattice and we show the distribution of the field intensity using a FDTD (Finite Difference Time Domain) method.

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