Simulation and design of photonic crystal with nonlinear components

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ABSTRACT

Nonlinear optical phenomena provide a physical mechanism for converting the light frequency. This allows the generation of tunable light sources at wavelengths inaccessible with lasers, leading to many applications in fields such as spectroscopy, sensing, and light trapping. The Kerr effect is a promising nonlinearity as it means a near-instantaneous intensity dependent refractive index change. Because of the weakness of this effect strong field confinements are necessary, which are now possible in advanced structures such as photonic crystals. For this reason, the field of non-linear optics in photonic crystals (PCs) presents a strong interest for photonic applications and all-optical signal processing. In the proposed work, we have developed a numerical approach based on Finite Difference Time Domain (FDTD) method to simulate light propagation through one-dimensional nonlinear photonic crystal structures with Kerr – type nonlinearity. Our developed nonlinear FDTD code was used to investigate the localization properties of the field modes. By analyzing the defect mode of symmetrical structure 1D PC it is shown that the full-width at half-maximum (FWHM) of the defect mode depends not only on the number of symmetry layers of 1D PC but also on refractive index and optical thickness of defect layer. The change of refractive index of defect layer causes the frequency shift of defect mode. In addition, we found, in the case of 1D PC with nonlinear central layer, that a bound mode is created inside the PBG of the perfectly periodic structure. The FWHM of the bound mode is decreased by increasing the input intensity which indicated a strong confinement of the light modes in such structure. It is also demonstrated that when the FWHM of defect mode is small enough and frequency of incident light and linear refractive index are selected carefully, a relatively low threshold optical bistability is able to be obtained.

Keywords: Nonlinear optical, physical mechanism, light frequency, spectroscopy, sensing, and light trapping

Introduction

The control of electric and magnetic properties of materials has been and still one of the major research areas nowadays. Studies on semiconductor physics have thus initiated the revolution of transistor technology 60 years ago. Meanwhile, the developments of technological processes on semiconductor such as growth of materials have made possible the manufacture of devices to control the propagation of the electrons and led to the explosion in the field of microelectronics. However, miniaturization of these objects seems reach their limits given the fact that it is accompanied by the increase of the internal resistances of the circuits which raises heat dissipation problems. In recent years, the scientific community began searching for an alternative to electronic circuits, and proposed the use of photonic circuits. These photonic circuits using light instead of electron as information carrier, provide the possibility to transmit higher-speed data while suppressing the heat dissipation problems and allowing for miniaturization in the micrometer and nanometer scales. To design such devices, one must be able to produce materials in which the propagation of light is controlled: these materials should provide the ability to prevent or allow, in certain frequency ranges, the propagation of light in one or more directions and/or the location of the light at other frequencies.

In this context, the use of structures having a periodic dielectric permittivity in one or more directions of the space has been proposed to control the propagation of electromagnetic waves. In the same way that the periodicity of a solid crystal governed energy bands and the electron conduction

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properties, a periodic structure in the scale of the wavelength of the dielectric materials makes it possible

to achieve engineering dispersive properties of the material. By analogy with the solid crystals, these

periodic structures are called photonic crystals (PCs). These structures are now the source of numerous

optical experiments such as inhibition of the spontaneous emission (Pottage et al., 2001; Noda et al.,

2000), the high-reflective omnidirectional mirrors and waveguides with low losses or alternatively,

original refractive properties light such as autocolimation or negative refraction (Prasad et al., 2003;

Lupu et al., 2004; AbdelMalek et al., 2005, 2007; Belhadj et al., 2005, 2007). It may be noted that

photonic crystals exist in nature. Fig. 1-1a shows an electron microscope picture of a natural opal

composed of a periodic lattice of the silica beads. This periodic arrangement of the silica beads is

responsible for the brilliant colors of natural opals; insofar the periodicity of the structure leads to

diffraction effects governed by Bragg law. Opal is not the only example of natural photonic crystal.

Australian and British biologists from Sydney and Oxford Universities have found a marine worm with

thorns that are more efficient photonic crystals as those manufactured in laboratories until now (Fig.

1-1b). We can find other examples of photonic crystals in nature as the wings of certain butterflies (Fig.

1-1c) or the peacock feathers (Fig. 1-1d).

The applications envisaged for these photonic crystals have, despite manufacturing, modeling

and characterization problems, far exceeded the initial idea of the control of spontaneous emission

(Yablonovitch, 1887). Today they cover a wide range going from the study of the strong coupling

atom/cavity to optical interconnects and logic gates (Saidani et al., 2012, 2015). Among these areas of

study we mention research conducted on the use of photonic crystals for nonlinear optics.

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many applications in fields such as spectroscopy, sensing, and light trapping. The Kerr effect is a

promising nonlinearity as it means a near-instantaneous intensity dependent refractive index change.

Because of the weakness of this effect strong field confinements are necessary, which are now possible

in advanced structures such as photonic crystals. For this reason, the field of non-linear optics in

photonic crystals presents a strong interest for photonic applications and all-optical signal processing

(Soljačić and Joannopoulos, 2004). The existence of numerous non-linear phenomena such as two-

photon absorption, third-harmonic generation, four-wave mixing, optical bistability, stimulated Raman

scattering has been demonstrated in photonic crystals by different groups (Tanabe et al., 2005; Monat

et al., 2009; McMillan et al., 2010; Yu et al., 2014).

The aim of this work is to develop a numerical approach based on Finite Difference Time Domain

(FDTD) method to simulate light propagation through one-dimensional nonlinear photonic crystal

structures with Kerr – type nonlinearity.

Result and Discussion

The propagation of light through photonic band gap (PBG) structures has been widely studied

in recent years (Joannopoulos et al., 1995; Soukoulis, 1993, 1996). An essential property of these

structures is the existence of a frequency band gap in which light propagation is prohibited. This is

analogous to the electronic band gaps in semiconductor crystals. In such a crystal, a moving electron

experiences a periodic potential generated by the atomic lattice, which produces a gap (forbidden

region) in the electronic energy band. This gap splits the energy band into two parts; the valence band

(the lower energy band) and the conduction band (the higher energy band). The optical analogy is the

photonic crystal where the periodic potential is due to a lattice of different refractive index media.

However, when a defect layer is introduced into a PBG structure, it can create donor or acceptor modes

in the photonic band gap (Yablonovitch et al., 1991). Similar to the case of an electron being localized

around a defect crystal, there is a significant field enhancement in the optical defect structure.

When Kerr nonlinearity is introduced in the PBG structures (the effective refractive index now

depends on the field intensity) it will alter the transmission spectrum including the position of the band-

edges. This dynamic shifting of the band-edges can produce optical bistability phenomena (Scalora et

al., 1994; Tran, 1996; Wang et al., 1997).
I- Linear properties of one – dimensional (1D) photonic crystal

In this section, we are interested in studying the photonic band gap characteristics of one-dimensional photonic crystal (1D PC). The 1D photonic band gap (PBG) structure consists of alternating layers with high refractive index \( n_H \) and low refractive index \( n_L \). The period of the 1D PBG structure is "\( a \)" and the thicknesses of the high and low refractive index layers are \( d_H \) and \( d_L \) respectively (see Fig. 1).

\[
a = d_H + d_L
\]

**Fig. 1:** Schematic diagram 1D photonic band gap (PBG) structure.

The simulation is a very helpful tool to study the influence of the different parameters of the 1D PBG structures on the transmission spectrum. These parameters are:

**I. 1. Refractive index ratio \( n_H/n_L \)**

This ratio influences on the width and the sharpness of the photonic band gap. The increase of the ratio \( n_H/n_L \) leads to the widening of the bandgap. This effect can be observed in Fig. 2, where the reflectivity spectra of three PC structures composed of 8 layers with different \( n_H/n_L \) ratio show a bandgap with different widths. We can also observe that the band edges become sharper when the ratio increases. It can be also noted that the PBG shifts toward lower frequencies as the \( n_H \) increases.

**I. 2. Number of periods of 1D PC structure**

The number of periods (\( N \)) influences on different characteristics of the photonic bandgap. The increase in the number of periods \( N \) leads to an increase of the reflectivity within the bandgap, and enlarges its width. The band edges also become sharper. Fig. 3 shows the reflectivity spectra of four 1D PBG structures with \( n_H = 2.0 \), \( n_L = 1.4 \) and different number of periods \( N \). We can observe that when \( N \) increases, the band edges of the filter are sharper and the reflectivity tends to the unity exponentially with \( N \) (Lekner, 2000).

**I. 3. Thicknesses of the layers**

Fig. 4 shows that when the thickness of the high refractive index layer "\( d_H \)" increases (i.e. \( d_L \) decreases) the PBG is shifted toward the low frequency region. It can be also noted that the width of the PBG is significantly decreased by increasing \( d_H \).

**II. Optical properties of linear PBG structure with a defect: Microcavities**

It is possible to create a photonic crystal microcavity by introducing a defect layer in 1D PBG structure (see Fig. 5). When a defect layer is introduced in 1D PBG structure, a very narrow resonance (also called transmission peak) that is isolated in the band gap occurs. The frequency of such resonance
is called a defect mode frequency. This is in contrast with the case of strictly periodic structure where all resonances are concentrated at the border or outside the band gap.

Fig. 2: Spectra of three different 1D PCs with 8 periods. The thickness of the layers are \( d_H = 0.3a \) and \( d_L = 0.7a \). The \( n_H/n_L \) ratio is: (a) 1.75/1.25, (b) 2/1.25, (c) 2.5/1.25.
Fig. 3: Reflectivity spectrum of 1D PC structure with $n_H=2.0$ $n_L=1.4$ and number of periods $N=4, 6, 8$ and 12.

Fig. 4: Reflectivity spectrum of 1D PC structure with $n_H=2.0$, $n_L=1.4$ and thickness of the high index layer of $d_H=0.34a$, $0.48a$ and $0.66a$. 
For convenience, we indicate the 1D-PC structure as \( (HL)^N D M (LH)^N \), where H indicates high dielectric layer with refractive index \( n_H \), L the low dielectric layer with refractive index \( n_L \) and D the defect layer with refractive index \( n_D \), respectively. \( N \) is the number of couple of layers with high and low refractive index, \( M \) is a multiple of the defect layer with an unit optical thickness of \( \lambda_0/4 \) and here \( \lambda_0 \) is the designed wavelength. Usually \( N \) is an integer while \( M \) can be chosen as a noninteger number.

In Fig. 6 we plot the transmission spectrum of a \( (HL)^4 D^2 (LH)^4 \) PC structure. From this figure we note that the structure has a transmitted frequency inside the PBG. This transmitted frequency is related to the defect layer and it is called defect mode or cavity mode.

**Fig. 5:** Schematic diagram 1D PC structure with defect \( (HL)^N D M (LH)^N \).

**Fig. 6:** Transmission spectrum of 1D PC microcavity with \( n_H = 2.5, n_L = 1.25 \) and number of periods \( N = 4 \). The thickness and the refractive index of the defect layer are \( d_D = 2a/3 \) and \( n_D = n_H \) respectively.
II. 1- Influence of the microcavity parameters

In a microcavity, the frequency at which resonant peak is located, its width and its reflectivity level depend on different parameters. In the following paragraphs we discuss the dependence of the defect modes on the thickness, the position and the refractive index of the defect layer and the number of layer periods.

II. 1. a- Thickness of the defect layer

First we study the influence of the defect thickness on the defect mode. It is well known, according to the theory of interference filter, that if the optical thickness of defect layer is \( \lambda_0/2 \) or \( \lambda_0 \), it has no effect on transmittivity of the defect mode. However, from the numerical result one can see that it affects band-gap width and the full-width at half-maximum FWHM of the defect mode.

Here we consider 1D PC structures (HL)^4(D)^4(LH)^4 with \( M=2, 4, 6 \) and \( 10 \) which correspond to defect thicknesses of \( d_D=\lambda_0/2, \lambda_0, 3\lambda_0/2 \) and \( 5\lambda_0/2 \) respectively. The transmission spectra of the considered structures are compared in Fig. 7. From this figure we can conclude that the FWHM of defect mode is narrowed by increasing the optical thickness of the defect layer. Such a phenomenon can be interpreted qualitatively by using the theory of Fabry-Perot interferometer.

![Fig. 7: Transmission spectrum of 1D PC microcavity for different defect layer widths. The refractive indices of the high index, low index and the defect layers are \( n_H=2.5, n_L=1.25 \) and \( n_D=n_H \) respectively.](image)

II. 1. b- Refractive index of the defect layer

Next we investigate the dependence of the defect mode on the refractive index of the defect layer. The property of defect mode in 1D-PC structure will be changed if refractive index of the defect
layer is modified in the condition of its optical thickness fixed. Take 1D-PC with structure (HL)⁴D⁴(LH)⁴ as an example. The optical thickness of defect layer is fixed at \(\lambda_0/2\) while the refractive index of the layer is varied so that physical thickness of the layer is changed accordingly.

![Transmission spectrum of 1D PC microcavity](image)

**Fig. 8:** Transmission spectrum of 1D PC microcavity (HL)⁴D⁴(LH)⁴ for different refractive index of the defect layer. The optical thickness of the defect layer is kept unchanged (=\(\lambda_0/2\)) but the physical thickness is changed.

The corresponding numerical simulation result is shown in Fig. 8 for three different refractive indices of defect layer \(n_D\). It is obvious that the full-width at half-maximum (FWHM) of defect mode decreases with the increase of refractive index of defect layer.

**II. 1. c- Position of the defect layer**

Now we study the influence of the defect position in the structure on the defect mode. We consider a structure of 9 alternating layers including 5 \(H\) layers and 4 \(L\) layers. The defect layer is introduced by changing the size of one of the layer \(H\) to be \(\lambda_0/2n_H\). The effect of defect position is investigated by moving the defect layer from the left to the right of the structure. The transmission spectra of the considered structures are compared in Fig. 9. From this figure it is found that the changing of the defect position disturbs the positions of the transmission maxima outside the band gap.

We also studied the effect of the position of the defect layer on the FWHM of the defect mode. Fig. 10 shows the FWHM of the defect mode for several defect layer positions. It can be easily noted from this figure, that the full-width at half-maximum (FWHM) of the defect mode increases when the defect layer is moved away from the middle of the structure.
Fig. 9: Transmission spectrum of 1D PC microcavity for different position of the defect layer. The optical thickness of the defect layer is $\lambda_0/2$.

Fig. 10: Profile of defect mode of 1D PC microcavity for different position of the defect layer. The optical thickness of the defect layer is $\lambda_0/2$. 
II. 1. d- Number of periods of the 1D-PC

Finally we investigate the effect of the number of layer periods on the defect mode properties. We consider the symmetrical 1D-PC structure (HL)^N(D)(LH)^N for N = 4, 5, 6, 7. The index and the optical thickness of the defect layer are chosen to be n_H and λ_0/2, respectively. Using this structure, a resonant mode in the center of the band gap of the corresponding perfect structure can be found. Fig. 11 shows the profile of the defect mode of the structure for different number of layer periods N. The spectral width FWHM of the defect mode is changed as the number of layer periods N changes. As larger N increases the FWHM of the defect mode decreases. More precisely, increasing the number of grating periods N yields a narrower resonance.

III- Behaviors of one-dimensional nonlinear photonic crystals

III. 1. Transmission properties of perfect nonlinear PBG structure

First, we examine the impact of third order optical nonlinearity on the photonic band gap of 1D PC structure. The one dimensional nonlinear structure 1D NPC considered consists of (HL)^8. We assume a Kerr nonlinearity with \( \chi^{(3)} = 2 \times 10^{-12} \) m^2 V^{-2} is present in all high index layers(Suryanto et al., 2003). Fig. 10 shows the transmission spectra of the 1D PC structure in the linear regime (solid line) and 1-D NLPC (solid line) calculated with the FDTD method. In the nonlinear case, the results are presented for several values of input intensity I_{inc}. As can be seen from Fig. 12, for the selected values of the input intensity the PBG of the 1D NPC structures is red-shifted (toward lower frequencies). This red-shift is in good agreement with Maksymov et al. (2004). For the 1-D NLPC, the red-shift can be explained with Scalora’s argumentation (Scalora et al., 1994). Since the dielectric constant depends on the field intensity, the transmission spectrum will also change dynamically with the incident field.

In fact, for the Kerr-nonlinear medium (the layers with a high dielectric constant), the dielectric permittivity is related to the electric field and the Kerr coefficient \( \chi^{(3)} \) by the relation (Lidorikis et al., 1996);

\[
\varepsilon(\vec{r},t) = \varepsilon_\infty + \chi^{(3)} |E(\vec{r},t)|^2.
\]
In the frequency domain, the band gap is determined by the difference between the dielectric permittivities of the materials, which form the photonic crystal. From Eq. (1), we can express this difference as:

$$\Delta \varepsilon = \varepsilon_H - \chi^{(3)} \left| E(\mathbf{r}, t) \right|^2 - \varepsilon_L.$$ (2)

The value of $\Delta \varepsilon$ increases as the intensity increases if $\chi^{(3)} > 0$ and decreases if $\chi^{(3)} < 0$. As the source excites the structure, the value of $\Delta \varepsilon$ changes and the bands of the band structure dynamically shift. This process is the basis for intensity-driven optical limiting and all-optical switching [73]. The results show that for the positive Kerr coefficient the value of $\Delta \varepsilon$ increases and the transmission spectrum dynamically red-shift. This red-shift increases as the intensity of the source increases.

For example, as can be seen from Fig. 12, for an input intensity of $I_{inc1} = 3 \times 10^2$ kW the transmission spectrum is just slightly shifted. While an input intensity of $I_{inc1} = 30 \times 10^2$ kW (ten-time increase in the input intensity), in fact, significantly shifts the spectrum.

**Fig. 12:** Transmission spectra of linear (solid line) and nonlinear 1D PC structures (HL)$^8$.

### III. 2. Transmission properties of 1D PC structure with a nonlinear central layer

In the previous section, we studied the impact of third order optical nonlinearity on the photonic band gap of 1D PC structure. In this section, we investigate the transmission behaviors of 1D PC structure with nonlinear central layer. The structure considered in this section has the form (HL)$^N$ (D) (LH)$^N$. We assume that Kerr nonlinearity is present in the central layer D.

First, we consider an 1D PC structure (HL)$^4$ (D) (LH)$^4$ in which we assume that only the central layer (defect layer D) has $\chi^{(3)}_D = 2 \times 10^{-12}$. The linear part of the refractive index of the Layer D is $n_D = n_H$.

Fig. 13 shows the transmission spectra of (HL)$^4$ (D) (LH)$^4$ structure for a linear and nonlinear central layer. From this figure it can be seen that when the central layer is linear, the structure looks to
be periodic and it exhibits a typical photonic band gap falling at the frequency range 0.227 to 0.372 \((a/\lambda)\). By replacement of the central layer with Kerr nonlinear impurity, the periodicity of the structure is altered and hence a bound mode is created inside the PBG of the perfectly periodic structure. As seen in the figure, the transmission peak of the bound mode is very narrow and occurred at normalized frequency 0.3359 \((a/\lambda)\). Such structure of bound mode can be used as the resonant cavities.

![Fig. 13: Transmission spectrum at normal incidence of 1D photonic crystal structure (HL)^3 (D) (LH)^4.](image)

The central layer is assumed to be nonlinear and the input intensity is \(I_{inc}=30.10^{2} \text{ kW}\).

Next, we study the effect of the input intensity on the bound mode characteristics. In Fig. 14 we plot the transmission spectra of the considered structure for different input intensities. The figure clearly shows that the increase of the input intensity shifts the frequency of the mode toward lower frequencies (red-shift). It can be also noted that the FWHM of the bound mode is decreased by increasing the input intensity.

III. 3- Bistability controlled by input intensity of 1D nonlinear PC structure

In this paragraph, we investigate the bistability behaviors of 1D NPC structure with defect. The defect structure considered in this section has the form \((HL)^N (D)^M (LH)^N\). We assume a Kerr nonlinearity with \(\chi^{(3)} = 2 \times 10^{-11} \text{ m}^2 \text{ V}^{-2}\) is present in all high index layers as well as in the defect layer. Here we calculate the complete relationship between the incident wave and transmitted wave intensities. When the input intensity is low, the defect mode frequency is assumed to be in linear state. However, if the input intensity is high, the refractive index of the defect layers increases and the frequency of the defect mode will be shifted to a lower frequency, as shown in Fig. 14.

In Fig. 15 we show the input-output characteristics of \((HL)^2 (D)^2 (LH)^2\) structure for an incident field frequency too close to the defect mode frequency \(\omega = 0.995 \omega_0\). It is clearly noted that the structure shows a bistability loop. When the incident intensity \(I_{inc}\) increases slowly from zero, the transmitted intensity \(I_{tr}\) first increases slowly. If the input intensity reaches the upswitching threshold value (about 785 kW/m^2), the transmitted intensity \(I_{tr}\) jumps to a higher value (from state 1 to 1’, see Fig. 15).
Fig. 14: Transmission spectra of $(HL)_4^2 (D) (LH)_4^2$ structure for different input intensities.

Fig. 15: Bistable loop of transmitted intensity as a function of incident intensity for $(HL)^2 (D)^2 (LH)^2$ structure with $n_D = n_H$ where the Kerr nonlinearity is introduced the defect layer. The input field has frequency $\omega = 0.995\omega_0$. 
Then $I_T$ increases slowly again as $I_{inc}$ increases. On the other hand, when $I_{inc}$ is decreased from the value that is greater than the threshold value, $I_T$ decreases slightly from the high state. When $I_{inc}$ reaches the threshold value (state 1'), $I_T$ does not jump back to lower value (state 1), but it remains to decrease slightly until it reaches state 2, at which it jumps to state 2'. Then $I_T$ continues to decrease with decreasing $I_{inc}$. Thus, the nonlinear defect structure can implement an optical bistability.

It should be noticed that the line between the low-output state and high-output state, i.e. the line which connects the state 1 and state 2, corresponds to the unstable solutions.

While the threshold value for $\omega = 0.995\omega_0$ is relatively large, this value can be reduced by tuning the frequency of the input light closer to the defect mode frequency. For example, the threshold values for frequencies $\omega = 0.996\omega_0$ and $\omega = 0.997\omega_0$ are 593 kW/m² and 437.5 kW/m² respectively. However, the bistable loop cannot be obtained anymore when the input field has frequency that is very close to the resonance frequency, e.g. in the case of $\omega = 0.9995\omega_0$, (see Fig. 16).

![Fig. 16: Bistable loop of transmitted intensity as a function of incident intensity for (HL)² (D)² (LH)² structure with $n_D = n_H$ for different input field frequencies where the Kerr nonlinearity is introduced the defect layer.](image)

References


