Analysis of photonic crystals for light emitting diodes using the finite difference time domain technique

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ABSTRACT

The Finite Difference Time Domain method has been used to analyze the dispersion diagram of a photonic crystal comprised of a perforated dielectric slab and the properties of a micro-cavity formed by introducing a defect into such a crystal. Computational requirements of the method, its advantages and disadvantages, and results for the structure analyzed are discussed.

1. INTRODUCTION

Structures with periodic modulation of the refractive index in two or three dimensions, or photonic crystals[1,2], exhibit interesting optical characteristics, not yet available with ordinary materials. When properly designed, photonic crystals may change significantly the way electromagnetic waves propagate: entire frequency bands or selected directions can be forbidden, and modes can be localized around defects in the crystal lattice[3]. At optical frequencies, these properties may be exploited to achieve, by the suitable design of the structure, performances not available with standard design techniques because of losses. In particular, there are research efforts toward the usage of photonic crystals to realize high efficiency or high-speed resonant-cavity light emitting diodes[4,5] for applications in telecommunications.

Many efforts have been devoted to the experimental verification of the properties of photonic crystals as well as to the development of suitable geometric configurations and of the nanofabrication technology needed for their realization at optical frequencies. A smaller amount of work has concerned the numerical analysis, and most of it has been done using the plane wave expansion method[6], which presents some convergence problems and can deal with the presence of a defect only by resorting to the computationally intensive super-cell approach. Only recently some well established methodologies, more flexible than the plane wave expansion method, have been adapted to the periodic geometry and applied to the analysis of photonic crystals. Among these, the Finite Element Method[7] and the Finite Difference Method both in Frequency (FDFD) [8] and in Time Domains (FDTD)[9] have been applied to practical cases.

In this paper, the application of the Finite Difference Time Domain method with a combination of periodic and absorbing boundary conditions to the computation of dispersion diagrams is outlined referring to the case of a perforated dielectric slab with a finite thickness. The method is also used with absorbing boundary conditions only to characterize the resonant modes of a micro-cavity formed by a defect introduced in the periodic structure.

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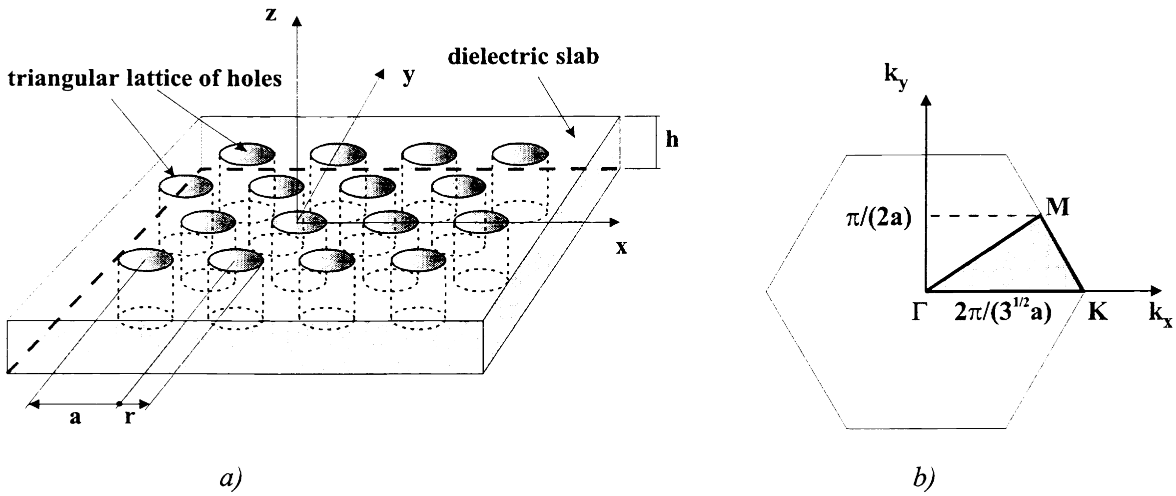

Fig. 1 – a) Dielectric slab with a triangular lattice of holes; b) Irreducible Brillouin zone for a triangular lattice.

2. NUMERICAL ANALYSIS

A. DISPERSION DIAGRAM

Calculation of the dispersion diagram implies consideration of the propagation of the electromagnetic wave in the infinite space tiled with identical cells. At a fixed instant of time, the only difference between the eigenmode's fields at corresponding points in different cells is the phase. Consequently, the computational domain may be restricted to a single unit cell of the crystal by enforcing appropriate periodic Bloch conditions at the boundary of the unit cell, and the problem can be solved by using the FDTD to solve the time-domain Maxwell's equations in the unit cell. The periodic structure under test is excited with either some initial electromagnetic field distribution or with a localized Gaussian pulse in time, and the marching-in-time scheme is applied to compute the electromagnetic field in the computational domain. If a localized source is used (a dipole in our case) to excite the structure, its spectrum must be wide enough to cover the frequency range of interest. Since periodic boundary conditions are applied, the electromagnetic field will reach a steady state after some time, and its spectrum will contain peaks at frequency values corresponding to the eigenmodes compatible with the wave vector $\mathbf{k}$ chosen to enforce the periodic boundary conditions. To show in detail how the method works, let's consider the case of a thin dielectric film with a triangular lattice of holes (Fig. 1a). The computational domain for the solution of Maxwell's equations is the single unit cell in real space shown in Fig. 2, and the dispersion diagram can be computed by varying the propagation vector along the edges of the irreducible Brillouin zone. In the case of a triangular lattice with lattice constant a, the irreducible Brillouin zone in the wave vector space is the shaded twelfth of the hexagon with side $4\pi/(3a)$ shown in Fig. 1b.

The computational domain shown in Fig. 2 is excited with a modulated Gaussian pulse and is terminated using Bloch boundary conditions at the lateral surfaces $x = \pm a/2$, $y = 0$, and $y = a\sqrt{3}/2$, while Absorbing Boundary Conditions

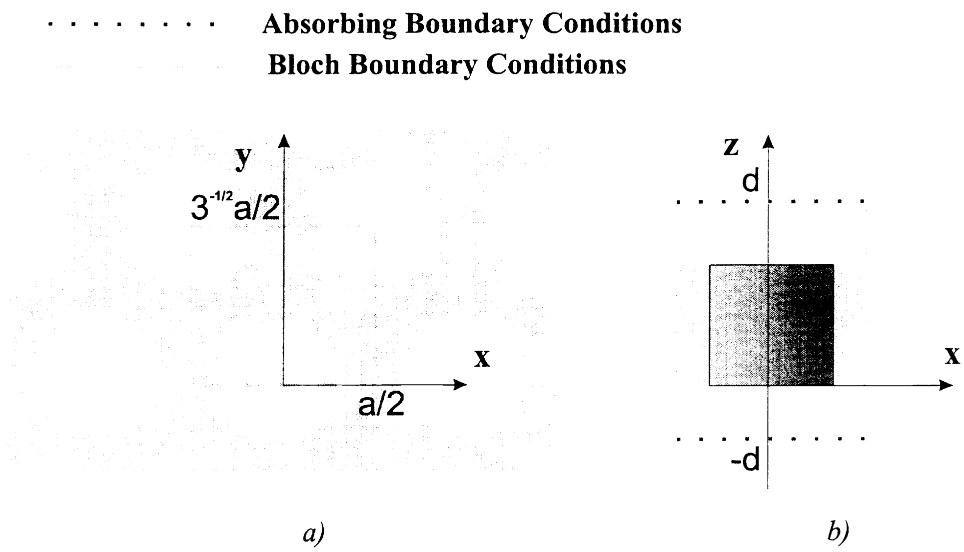

Fig. 2 – Computational domain in the real space for the computation of the dispersion diagram and boundary conditions used to terminate it. *a)* Top view; *b)* side view.

(ABC) are employed at the surfaces $z = \pm d$. By enforcing the periodic boundary conditions, one fixes a point in the wave vector space. As a matter of fact, the periodic boundary conditions include the wave vector $\mathbf{k}$, and can be expressed in the frequency domain as:

$$\mathbf{E}(\mathbf{r}+\mathbf{R},t) = \mathbf{E}(\mathbf{r},t)e^{-j\mathbf{k}\cdot\mathbf{R}} \qquad \mathbf{H}(\mathbf{r}+\mathbf{R},t) = \mathbf{H}(\mathbf{r},t)e^{-j\mathbf{k}\cdot\mathbf{R}} \tag{1}$$

with $\mathbf{R}$ standing for a lattice constant vector.

The implementation of the above relations in the time domain may be done in different ways, but to have stable results it is convenient to introduce two electromagnetic fields[10], having time dependence sin(ωt) and cos(ωt), that will be denoted with $[\mathbf{e}_1(x,y,z;t), \mathbf{h}_1(x,y,z;t)]$ and $[\mathbf{e}_2(x,y,z;t), \mathbf{h}_2(x,y,z;t)]$, respectively. Then, the periodic boundary conditions in equation (1) may be written in the time domain as:

$$\mathbf{e}_1(\mathbf{r}+\mathbf{R};t) = \mathbf{e}_1(\mathbf{r};t)\cos(\mathbf{k}\cdot\mathbf{R}) - \mathbf{e}_2(\mathbf{r};t)\sin(\mathbf{k}\cdot\mathbf{R}) \tag{2}$$

$$\mathbf{e}_2(\mathbf{r}+\mathbf{R};t) = \mathbf{e}_1(\mathbf{r};t)\sin(\mathbf{k}\cdot\mathbf{R}) + \mathbf{e}_2(\mathbf{r};t)\cos(\mathbf{k}\cdot\mathbf{R}) \tag{3}$$

$$\mathbf{e}_1(\mathbf{r};t) = \mathbf{e}_1(\mathbf{r}+\mathbf{R};t)\cos(\mathbf{k}\cdot\mathbf{R}) + \mathbf{e}_2(\mathbf{r}+\mathbf{R};t)\sin(\mathbf{k}\cdot\mathbf{R}) \tag{4}$$

$$\mathbf{e}_2(\mathbf{r};t) = -\mathbf{e}_1(\mathbf{r}+\mathbf{R};t)\sin(\mathbf{k}\cdot\mathbf{R}) + \mathbf{e}_2(\mathbf{r}+\mathbf{R};t)\cos(\mathbf{k}\cdot\mathbf{R}) \tag{5}$$

Certainly $\mathbf{e}_1$ and $\mathbf{e}_2$ can be thought of as real and imaginary parts of the complex electromagnetic fields. These relations, together with the analogous ones for the magnetic field, allow updating the field at the periodic boundaries of the computational domain. It is also worth stressing that equations (2-5) introduce the direction of propagation and the value of

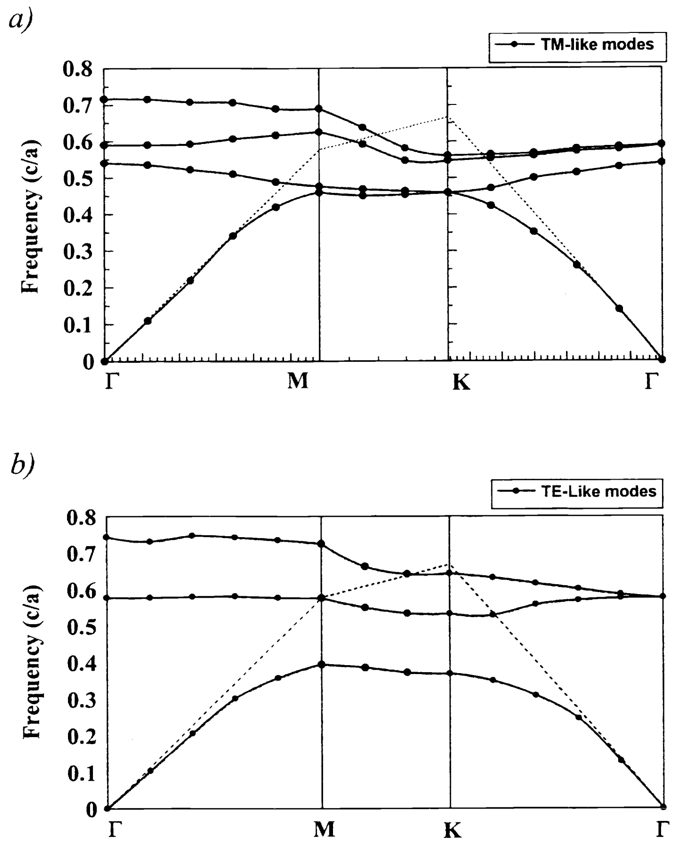

Fig. 3 – Dispersion diagram for a dielectric slab with a triangular lattice of holes. *a)* TM-like modes; *b)* TE-like modes.

the phase constant into the computations. For each value of the wave vector **k**, which is normally chosen along the edges of the Brillouin zone, the Maxwell's equations are solved and the field is observed at some points of the computational domain. Such observation points are placed out of symmetry planes for the lattice to avoid the possibility of probing the field in the null of the possible modes. The Fourier Transform of the computed signal has peaks at frequencies of the modes that can propagate in the structure with a given value of the wave vector **k**.

B. MICROCAVITIES

Introduction of an irregularity in the photonic crystal, often referred to as a defect, may cause localization of one or more electromagnetic modes around the defect itself. The FDTD algorithm with absorbing boundary conditions on all boundaries of the computational domain is applied to analyze these cavity modes and to determine their resonant frequency and Q.

The Fourier transform of the electromagnetic field at observation points inside the cavity gives the resonant frequencies of the cavity, while the Q of each mode can be estimated from the decay rate of the energy stored in the cavity. Modeling of the cavities takes much more computer memory than calculation of the dispersion diagram because of the bigger computational domain, while the number of time steps needed to reach a steady state is approximately the same.

It can be shown that in order to achieve high efficiency the resonant mode of a cavity-enhanced light emitting diode must be localized as tightly as possible while its Q must be approximately equal to that of the active material[11]. A Figure-of-Merit for the cavity optimization is the mode's effective volume normalized to the cubic wavelength of the resonant mode λ_0:

$$f = \frac{\int \varepsilon(\mathbf{r})\mathbf{E}^2(\mathbf{r})d^3\mathbf{r}}{(\lambda_0 / n)^3 \left(\varepsilon(\mathbf{r})\mathbf{E}^2(\mathbf{r})\right)_{\max}} \tag{6}$$

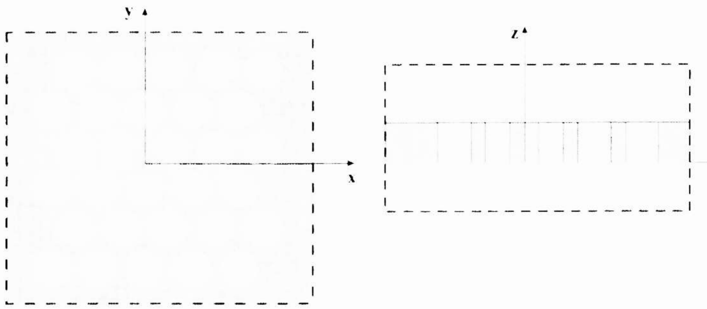

Fig. 4 – Defect realized by adding material in the bridge among three holes. The dotted line denote the boundary of the computational domain where ABC are enforced. *a)* Top view; *b)* side view.

The FDTD algorithm allows a straightforward computation of the effective volume of the cavity modes with the highest Q, that is the mode that survives after a sufficiently long waiting time, using Eq. 6.

Thus, we have tools to calculate resonant frequencies, field and energy distribution of resonant modes, as well as their Q and effective volume. All this information is necessary for a proper design of a cavity-enhanced light-emitting diode.

3. NUMERICAL RESULTS

The finite difference Time Domain method has been applied to the analysis of a triangular array of circular holes drilled in a thin dielectric slab. Wave propagation in such a structure was previously calculated using the plane wave expansion method[12] with the super-cell approach. Fig. 3 shows the dispersion diagram of the triangular array of holes in a dielectric slab with $\varepsilon_r = 12$ when the propagation vector $\mathbf{k}$ is varied along the border of the irreducible Brillouin zone (in-plane propagation). The ratio between the thickness h of the slab and the lattice constant a is $h/a = 0.5$, while $r/a = 0.45$ with

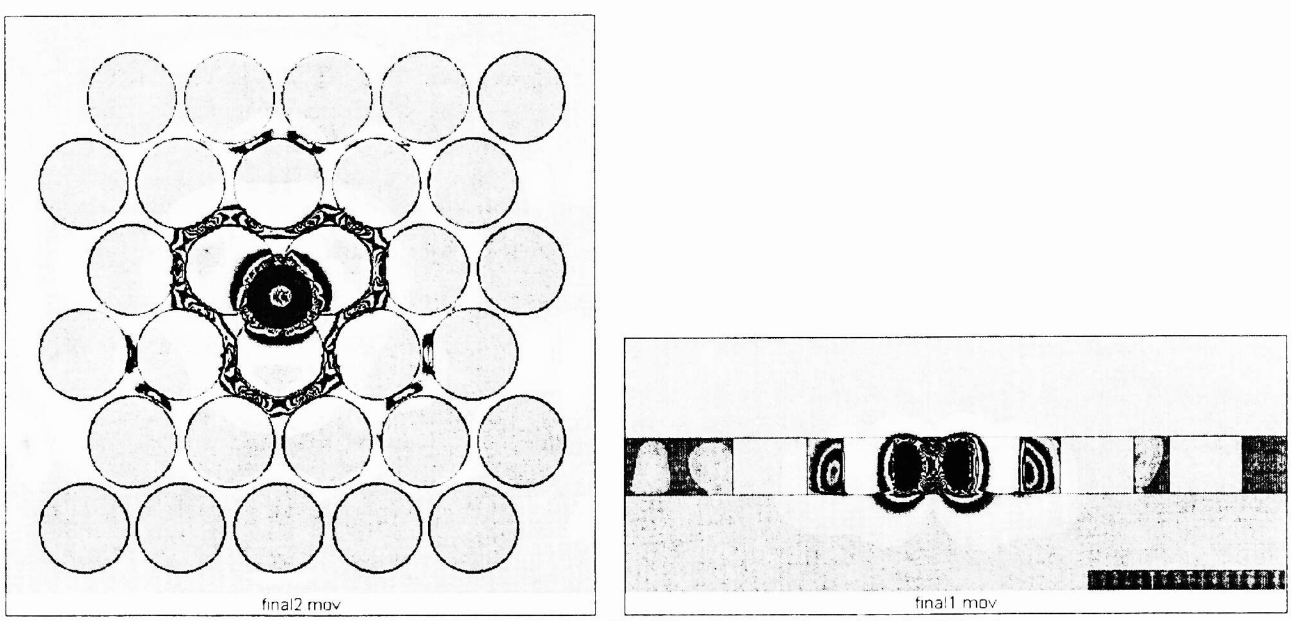

Figure 5 – Energy density distribution of the fundamental mode of the cavity. *a)* Top view; *b)* Side view.

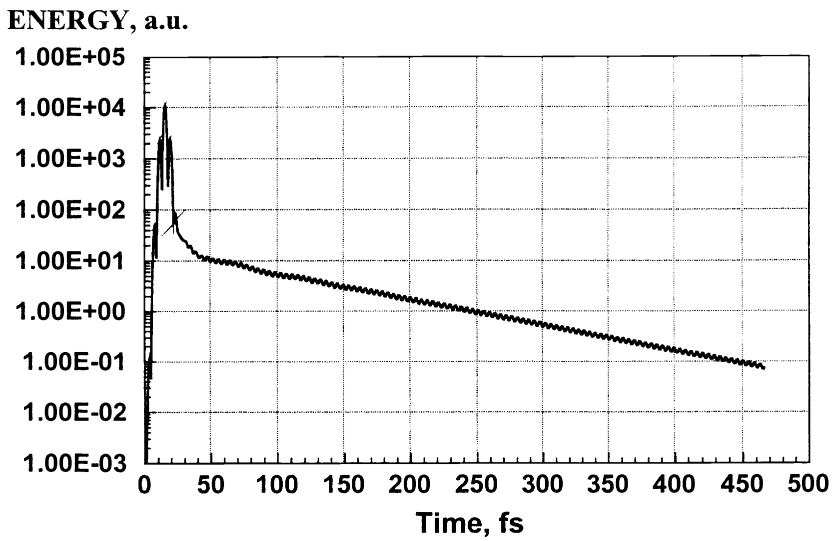

Figure 6 – Leakage of the energy stored in the cavity. The slope of the curve gives the cavity Q.

r being the radius of the holes. Our results for the two lower bands were within 5% of those reported in 12. A wide forbidden gap for the TE polarization exists in the range of normalized frequencies $0.37 \le a/\lambda \le 0.53$. This structure can be used as a reflecting medium to build a cavity. In the following, we consider a more realistic structure where the semiconductor slab is placed on a glass substrate with refractive index n_g=1.5.

A traditional way of creating a defect is to omit one hole. However, this is not the most prospective way of creating a cavity since it does not give any tuning freedom, and produces rather big cavities. Instead, we studied modes created by adding some extra material to the bridge between two or three holes as in Figure 4. This structure can be described by three independent dimensionless parameters: normalized thickness t/a, normalized radius of the holes r/a and normalized size of the radius defect r_d/a. Therefore, optimization of the effective volume f has to be performed in the three-dimensional parameter space:

$$f(t/a, r/a, r_d/a) = \frac{\int \varepsilon(\mathbf{r})\mathbf{E}^2(\mathbf{r})d^3\mathbf{r}}{(\lambda_0/n)^3\left(\varepsilon(\mathbf{r})\mathbf{E}^2\right)_{\max}} \tag{7}$$

The energy distribution in the cavity after the steady state of the mode is reached, is shown in Fig. 5. It is evident that a mode with C_3 symmetry is tightly localized at the defect. The time dependence of the energy stored in the cavity, shown in Fig. 6, gives the mode's Q=60. Short time Fourier transform of the electric field in the cavity gives the normalized resonant wavelength λ_0/a=0.44, and the normalized cavity volume cavity volume $f = 2.1$.

We are currently working toward the optimization of the dimensions of the cavity to achieve maximum efficiency in terms of mode's effective volume and the Q of the mode.

4. CONCLUSIONS

We presented an FDTD technique to compute dispersion diagrams of two- and three-dimensional photonic crystals and to characterize localized modes supported by a defect in the crystal lattice. The dispersion diagram is calculated on the unit cell using a combination of periodic Bloch boundary conditions and absorbing boundary conditions. The resonant modes of the cavity, their effective volume and quality factor are evaluated employing a larger computational domain with absorbing boundary conditions only. A perforated slab with a defect in the periodic structure is shown to be a good candidate for the fabrication of a microcavity light-emitting diode, a novel optoelectronic device which may be a valuable component of telecommunication systems due to its high raw efficiency and higher modulation speeds.

5. REFERENCES

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