

## COMPUTER SIMULATIONS FOR LARGE BAND GAPS IN PHOTONIC CRYSTALS

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*Folosind simulări numerice, s-a proiectat un cristal fonic 2D acordabil cu benzi interzise. Rezultatele au arătat ca o configurație simplă de tip fagure realizată din materiale feroelectrice poate avea benzi interzise într-un interval larg de frecvențe, dacă constanta dielectrică este modificată corespunzător cu ajutorul unui câmp electric. Au fost făcute mai multe modelări, fiecare corespunzând la o altă valoare a constantei dielectrice, și s-au obținut diferite intervale de benzi interzise.*

*With the aid of computer simulations we design an accordable 2D photonic crystal with band gaps. Results show that a simple honeycomb configuration micromachined on ferroelectrics could have band-gaps in a large interval, if the dielectric constant is suitable changed by an appropriate voltage. Several runs were done for different values of the dielectric constant and different intervals of band – gaps were obtained*

**Keywords:** accordable photonic crystals, band gap.

### 1. Introduction

The pioneering work of Yablonovitch [1] and John [2], emphasized the analogy between electronic waves in a crystal and light waves in a three-dimensionally periodic structure, and evidenced a complete photonic band gap. In 1991, Yablonovitch [3] has demonstrated the first three-dimensional photonic band gap in the microwave regime.

Ferroelectrics have many remarkable properties, like nonlinear optical response, and this property can be widely exploited for designing tunable photonic crystals [4]. An external quasistationary electric field may cause substantial nonlinear response especially in the microwave range [5].

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Continuing a previous work [6], our aim is to design by computer simulations a accordable photonic crystal with complete band gaps in the THz frequency range.

## 2. Methodology

Calculation of the dispersion relation and the associated band gaps in an ideal photonic material is well understood. The periodicity of the medium allows the use of the Bloch's theorem, leading to an eigenvalue problem [7]. For the numerical solutions of the eigenvalue problem, we used the free available MPB package developed by Joannopoulos and associates.

As stressed by Joannopoulos et. al. [8], a 2D photonic crystal consisting in a honey-comb lattice of dielectric rods has a complete photonic band gap. If the lattice were to be micromachined into a ferroelectric, a voltage appropriately varied will induce large enough change in the dielectric constant, as to 'move' the band gap for to encompass a large range.

## 3. Results and discussion

In this paper we prove the possibility to tune the bandgap in the range of THz. The structure of bands calculated for a honey-comb configuration of ferroelectric rods for relative dielectric constant,  $\varepsilon = 7$  to  $\varepsilon = 150$  are presented in Table 1. One can observe that for each value of the dielectric constant a large bandgap exists.

Several runs were made with the MPB code, corresponding to  $\varepsilon$  belonging to the interval [7-150], but only the run corresponding to the  $\varepsilon = 7$  is shown in Fig. 1 below.

As can be seen from Table 1, where the results of seven representative runs are displayed, the system exhibits complete photonic band gaps covering the interval  $0.062 - 0.269$  (in  $c/a$  units, where  $c$  is the speed of light in vacuum and  $a$  is the lattice constant,  $a \cong 3\mu m$ ). Of course, the voltage applied to the structure must be appropriately modified in order to obtain the corresponding band gap, which is not so simply to realise in practise, because a field of several hundreds of V/cm must be applied, depending on the ferroelectric structure .

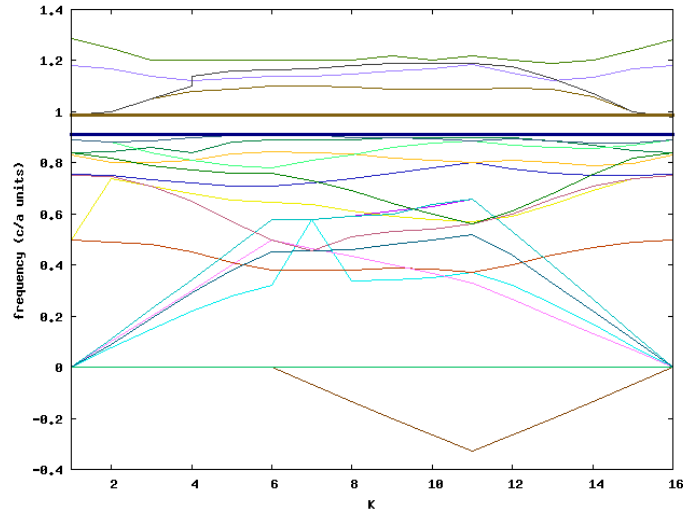


Fig.1: frequency (in c/a units) vs wave number k

In order to see if all the range of frequencies between  $6.2 \times 10^{12}$  Hz and  $2.69 \times 10^{13}$  Hz is covered, an evaluation of this bandgap on different values of relative dielectric constant is made. Fig. 2 shows the band – gap percentage as function on  $\epsilon$ . So, one can tune the bandgap of a structure with a given geometry only by modifying the dielectric constant of the material. The calculations also show that, for different values of the dielectric constant, the relative width of the bandgap is increasing from 13.2 % for  $\epsilon = 7$  to almost 42% corresponding to  $\epsilon = 150$ .

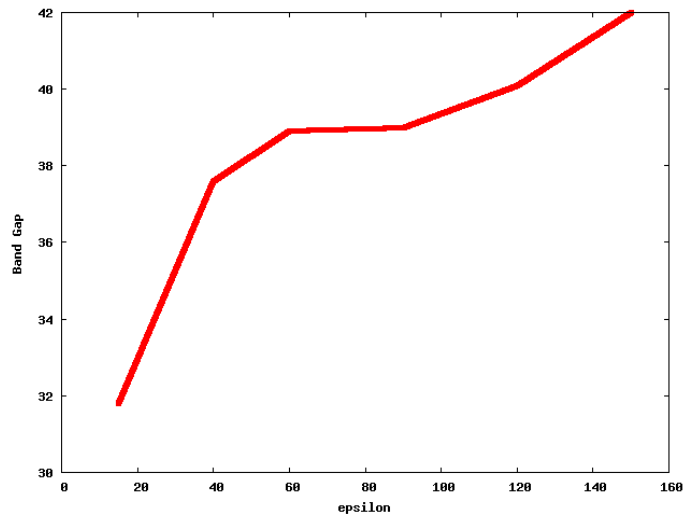


Fig. 2: Band gap percentage vs epsilon

Table 1

**Band Gaps as Function of Dielectric Constant**

Dielectric constant $\epsilon$	Band gap for $a \approx 3\mu m$ (in $c/a$ units)	Band gap (* $10^{12}$ Hz)	Band gap(%)
150	0.062 – 0.09	6.2 – 9.0	42.0
120	0.07 – 0.105	7 – 10.5	40.1
90	0.08 – 0.121	8 – 12.1	39.0
60	0.098 – 0.146	9.8 – 14.6	38.9
40	0.12 – 0.177	12 – 17.7	37.6
15	0.195 – 0.269	19.5 – 26.9	31.8
7	0.867 – 0.982	86.7 – 98.2	13.2

#### 4. Conclusions

We studied by numerical simulations the possibility of obtaining large band gaps in ferroelectrics. In this scope a 2D photonic crystal of ferroelectric rods was envisaged. The dielectric constant can be varied in practice by an external electrical field. For a lattice constant of about  $3\mu m$  and for a dielectric constant varying between 7 and 150, the range from  $6.2 \times 10^{12}$  Hz to  $2.69 \times 10^{13}$  Hz is covered with band gaps.

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