Effects of hydrostatic pressure on an L1 and L3 cavity of a photonic slab

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Abstract
In this work, we used the guided-mode expansion method to calculate the photonic band dispersion in two-dimensional photonic crystal slabs. The photonic lattice is hexagonal, composed of air holes with a circular cross-section. The slab is made of a semiconductor material (GaAs) with a dielectric function dependent on pressure and temperature. By maintaining the constant temperature, we found a shift in the photonic band dispersion towards regions of larger frequencies when the hydrostatic pressure increased. Moreover, we consider the effects of pressure on defective modes in cavities L1 and L3. The results reveal that by increasing the pressure, the position of the defective modes manages to tune for the photonic gap. Additionally, we found a decrease in the Q-factor for the L1 cavity when the pressure increases. However, for the L3 cavity, the Q-factor exhibits a non-monotonous behavior by increasing the pressure.

1. Introduction
The origin of photonic crystals (PC) was in 1987 via the works of E. Yablonovitch [1] and S. John [2], who proposed the use of structured materials with multi-dimensional periodicity to control light propagation. PCs are analogous to crystalline solids, which comprise the combination of atoms and the existence of an electronic band structure [3]. PCs are artificial structures with a macroscopic dielectric constant, which determines all the electromagnetic properties according to the equations of Maxwell’s electromagnetic theory [4]. In the photonic band dispersion, the frequency ranges where light propagation is not allowed are known as photonic gaps [5].

The existence of photonic gaps is one of the main characteristics of PCs; thus, it attracts considerable attention of researchers in important applications, such as superprisms [6, 7], photonic crystal fibers [8, 9], and optical cloaking [10, 11].

In one-dimensional PCs (1D-PC) the transfer matrix method (TMM) is used to calculate the shift exhibited by the long-wavelength transmittance spectrum in a structure composed of quartz-silicon [12], and nanocomposite [13] layers. In these structures, the Maxwell-Garnett model and Sellmeier approach are used to determine the dielectric constant. By altering the optical contrast of the constituent materials of the PC using external agents, such as temperature [14, 15] and hydrostatic pressure [16, 17], tuning the photonic band dispersion of the PC is possible. In the case of 1D-PC, a previous study showed that the photonic band dispersion shift is mainly caused by the optical response due to hydrostatic pressure [18]. By assuming the dependence of the dielectric function of GaAs on pressure and temperature [19], Segovia et al [20, 21] reported, the shift of the photonic band dispersion by increasing the pressure in a two-dimensional PC (2D-PC) comprising cylindrical holes arranged in a hexagonal and square lattice using the plane wave expansion method. The results revealed that by removing a hole of the lattice, the defective mode is tuned to higher frequencies when the pressure is increased. In [22], the combined effects of hydrostatic pressure and the size of the cross-sectional dispersers in the shape of equilateral triangles on the photonic band dispersion in a hexagonal lattice of the 2D-PC were investigated. They reported an increase in the width of the photonic gap by augmenting triangle lengths,
accompanied by a shift to high frequencies when the pressure increased. Recently, the effects of pressure on 2D-PC with a hexagonal lattice have become relevant for designing pressure sensors in megapascal to gigapascal operability ranges [23].

Currently, the research is aimed at confining light in the three spatial directions to the embedded 2D-PC in a planar waveguide, known as PC slabs [24]. In this type of structure, the photonic modes suffer a blue shift owing to the confinement to the vertical direction of the planar waveguide. In [25], the authors study the interaction between a PC slab and a multilayer supporting Bloch surface waves and report that the position and width of the PBGs are affected by the filling fraction. Hence, a wider PBG is associated with a reduction in the group velocity near the band-edge. Among the theoretical methods used to calculate the photonic band dispersion in PC slabs, we can mention the scattering-matrix [26, 27], finite-difference time-domain [28, 29] and guided-mode expansion (GME) [30]. Herein, we study the effects of hydrostatic pressure on the photonic band dispersion in a PC slab surrounded by air. This paper is structured as follows. In section 2, we present the theoretical GME model with the fundamental equations used to calculate the photonic band dispersion. In section 3, we present the numerical results for the regular and defective PC slab. Finally, in section 4, we present the conclusions.

2. Theoretical framework

In linear, isotropic, non-magnetic media and the absence of sources, the master equation for the magnetic field \( \vec{H}(\vec{r}) \) is given by

\[
\nabla \times \frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H}(\vec{r}) = \frac{\omega^2}{c^2} \vec{H}(\vec{r})
\]

(1)

where \( c \) and \( \omega \) are the velocity of light and angular frequency of the electromagnetic mode [31], respectively. In PCs, the dielectric constant is a periodic function, which conforms to \( \varepsilon(\vec{r}) = \varepsilon(\vec{r} + \vec{R}) \), where \( \vec{R} \) are the lattice vectors. The photonic band dispersion can be calculated using the GME method proposed by D. Gerace et. al [30]. In this method, the field \( \vec{H}(\vec{r}) \) expands on the basis of the guided modes, as follows:

\[
\vec{H}(\vec{r}) = \sum_{\mu} c_{\mu} \vec{H}_{\mu}(\vec{r})
\]

(2)

When replacing equation (2) in equation (1), we get a linear eigenvalue problem, which is given by

\[
\sum_{\mu} \mathcal{M}_{\mu\nu} c_{\mu} = \omega^2 c^2 c_{\nu}
\]

(3)

In equation (3), the matrix elements \( \mathcal{M}_{\mu\nu} \) are given by

\[
\mathcal{M}_{\mu\nu} = \int \frac{1}{\varepsilon(\vec{r})} \left[ \nabla \times \vec{H}_{\mu}(\vec{r}) \right] \cdot \left[ \nabla \times \vec{H}_{\nu}(\vec{r}) \right] d\vec{r}
\]

(4)

The basis for expanding equation (2) is determined by the homogeneous dielectric slab. In figure 1(a), the PC slab of interest is shown, which is formed by a hexagonal lattice (plano xy) of air holes patterned on a free-standing high-index slab of thickness \( d \). In figure 1(b), we represent the homogeneous planar waveguide in the vertical direction \( z \) with dielectric constants for the lower cladding (\( \varepsilon_1 \)), core (\( \varepsilon_2 \)) and upper cladding (\( \varepsilon_3 \)). By

![Figure 1](image-url)
applying continuity conditions of the tangential components of the transverse-electric fields (electric field $\mathbf{E}$ lies on the $xy$ plane) and the transverse-magnetic field ($\mathbf{H}$ lies on the $xy$ plane), to the waveguide problem, solutions are determined by the following implicit equations:

\[
q(\chi_1 + \chi_3) \cos(qd) + (\chi_1 \chi_3 - q^2) \sin(qd) = 0
\]

\[
\frac{q}{\tau_1} \left( \frac{\chi_1}{\tau_1} + \frac{\chi_3}{\tau_3} \right) \cos(qd) + \left( \frac{\chi_1 \chi_3}{\tau_1 \tau_3} - \frac{q^2}{\tau_2} \right) \sin(qd) = 0
\]

In equations (5) and (6), $\chi_1 = \sqrt{g^2 - \tau_1 \tau_2}$, $q = \sqrt{\tau_1 \tau_3} - g^2$ and $\chi_3 = \sqrt{g^2 - \tau_1 \tau_2}$. The wave vector of the $xy$ plane is represented by $\mathbf{g}$ with modulus $g$ and unit vector $\hat{g}$. Guided modes in the homogeneous dielectric slab (see figure 1(b)) depend on vector $\mathbf{g}$, whereas in the PC slab, the photonic modes are determined by the Bloch vector $\hat{k}$ restricted to the values in the first Brillouin zone of the hexagonal lattice. The expansion given by equation (2) can be written for the guided-mode basis as follows:

![Figure 2. Photonic band dispersion for a PC slab with hexagonal lattice of air holes. For a pressure of 0 kbar: (a) TE-like and (b) TM-like. (c) TE-like for $P = 0$ kbar (black line) and $P = 70$ kbar (dark blue line). The values used in the simulations are $T = 4$ K, $d = 0.5a$, and $R = 0.3a$. The blue region indicates the light cone, and the photonic gaps are represented in grey ($P = 0$ kbar) and orange ($P = 70$ kbar).]
where $\vec{G}$ is the reciprocal lattice vector in 2D, and $\alpha$ is a discrete index for labels of guided modes. In equation (4), we expand the dielectric function in a set of planes waves as follows:

$$\frac{1}{\epsilon(\vec{r})} = \sum_{\vec{G}} \eta_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$$

The Fourier coefficients $\eta_{\vec{G}}$ are given by

$$\eta_{\vec{G}} = \frac{1}{A} \int \epsilon^{-1}(\vec{r}) e^{-i\vec{G} \cdot \vec{r}} d^2r$$

where the integral extends over the unit cell of area $A$ and $\vec{r} = (x, y)$ [32]. Finally, the quality factor ($Q$) for a photonic mode with frequency $\omega_k$ can be calculated using the GME method by computing the imaginary part of the frequencies ($Im(\omega_k)$), as follows:

$$Q = \frac{\omega_k}{2Im(\omega_k)}$$

3. Results and discussions

In this paper, we focus our attention on a symmetric PC slab surrounded by air, $\tau_1 = \tau_3 = 1.0$. The hexagonal photonic lattice of air holes exists only inside the slab core, where the dielectric function of the slab is of a semiconductor material (GaAs) which depends on the hydrostatic pressure ($P$) and temperature ($T$), thus,

$$\epsilon_{GaAs}(P, T) = (\epsilon_0 + A e^{T/T_0}) e^{-\alpha P}$$

with $\epsilon_0 = 12.446, A = 0.21125, T_0 = 240.7$ K, and $\alpha = 0.00173$ kbar$^{-1}$ [19]. In the hexagonal lattice of circular cross-section air holes, the Fourier coefficients calculated by equation (9) are given by

![Figure 3. (a) Top view of the PC slab for the L1 cavity for $T = 4$ K, $P = 0$ kbar and $R = 0.3a$. (b) Photonic band dispersion for the TE-like mode, with the defective modes for $P = 0$ kbar (black dashed line) and $P = 70$ kbar (blue dashed line).]
where $a$ is the lattice constant, $R$ is the radius of the holes and $J_1(RG)$ is Bessel's first-class function.

In numerical simulations, to calculate the photonic band dispersion, we consider constant values of temperature ($4K$), slab thickness ($0.5a$) and radius of holes ($0.3a$). Because of the absence of translational symmetry in the $xy$ plane, the TE (transverse-electric) and TM (transverse-magnetic) pure modes are no longer separable. However, in a PC slab independent of symmetry, the modes can be classified mainly into two types: TE-like and TM-like. For a pressure of $0$ kbar ($\epsilon_{\text{GaAs}} = 12.66$), in figures 2(a) and (b), we present the photonic band dispersion using a dimensionless frequency ($\omega a/2\pi c$) for TE-like and TM-like modes, respectively. In figure 2, we note that the region in blue determines the light cone, and the discrete modes are vertically confined by the index confinement lying below the light cone (white region). For low frequencies in the photonic band dispersion of the TE-like modes, there is a photonic gap for the region within $0.259 \leq \omega a/2\pi c \leq 0.339$. Next, we will only focus on TE-like modes. The effects of hydrostatic pressure on the photonic band dispersion are presented in figure 2(c). As the pressure increases by 70 kbar, the dielectric constant of GaAs decreases ($\epsilon_{\text{GaAs}} = 11.21$), causing a shift of the bands to regions of larger frequencies with photonic gap constant located in $0.274 \leq \omega a/2\pi c \leq 0.356$.

When the periodicity of the 2D-PC is broken by the insertion (or removal) of impurities, defective modes originate inside the photonic gap allowing the location of the electromagnetic field around the defect. In figure 3(a), the top view of the PC slab is shown with the removal of an air hole (cavity L1) for $T = 4K$, $P = 0$.
kbar, and \( R = 0.3a \). Using the supercell technique, we find a defective mode within the photonic gap for the TE-like photonic band dispersion when \( P = 0 \) kbar, which is located in \( \omega a/2\pi c \approx 0.292 \). By increasing the hydrostatic pressure by 70 kbar, the defective mode changes position at larger frequencies and is now located at \( \omega a/2\pi c \approx 0.309 \), as shown in figure 3(b). Additionally, we evaluate the Q-factor in the L1 cavity using equation (10). We found a decrease in the Q-factor as the pressure increased. For values of 0 kbar and 70 kbar, the Q-factor is 399.517 and 215.548, respectively.

The tuning of the defective mode when increasing pressure for an L3 cavity (by the removal of three air holes) is presented in figure 4. In the photonic band dispersion for \( P = 0 \) kbar (see figure 4(a)), the existence within the gap of five defective modes located in \( \omega a/2\pi c \approx 0.269, 0.289, 0.292, 0.293 \) and 0.31 is shown. In this figure, it can be observed that the results agree to those reported in the scientific literature [33, 34].

Unlike the results presented for the L1 cavity where the Q-factor has a decreasing behavior with the increase in pressure, in an L3 cavity, the Q-factor has a non-monotonous behavior because some modes excited by increase pressure favor the increase of the Q-factor. In the L3 cavity for \( P = 0 \) kbar, the Q-factor is 5774.98 (mode 1), 759.122 (mode 2), 259.473 (mode 3), 525.661 (mode 4) and 510.777 (mode 5). In figure 4(b), we present the intensity \( |E|^2 \) for the modes of the L3 cavity for \( P = 0 \) kbar in symmetry point M \((k_x a = 0, k_y a = 2\pi/\sqrt{3})\). By increasing the pressure by 70 kbar, the position of the five modes changes to larger frequencies \( \omega a/2\pi c \approx 0.286, 0.307, 0.309, 0.311 \) and 0.3379, as shown in figure 4(c). The Q-factor of the five modes for 70 kbar is 6357.36, 478.431, 176.5, 169.54 and 530.308.

4. Conclusions

Using the GME method, we calculate the photonic band dispersion in a regular and defective PC slab (for L1 and L3 cavities). The PC slab is formed by a hexagonal lattice of air holes, where the dielectric function of the slab depends on the hydrostatic pressure and temperature applied. When keeping the temperature constant, we detected a shift to higher frequencies of the photonic band dispersion for TE-like modes. Additionally, we detected that in the case of the L1 and L3 cavities, within the photonic gap the defective modes are able to tune to higher frequencies when pressures are increased. For the L1 cavity, we reported a decrease in the Q-factor by increasing the applied pressure. However, for the L3 cavity, the Q-factor exhibits a non-monotonous behavior.

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