

# ACTIVE PHOTONIC CRYSTAL NANO-ARCHITECTURES

#### CHRISTOPHER J. SUMMERS, CURTIS W. NEFF and WOUNJHANG PARK

School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0245, USA

and

Department of Electrical & Computer Engineering, University of Colorado, Boulder, CO 80309-0425, USA

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The development of nano-scaled photonic crystal structures has resulted in many new devices exhibiting non-classical optical behavior. Typically, in these structures a photonic band gap and associated defect mode are used to create waveguides, resonators, couplers and filters. In this paper we propose that the functionality of these structures can be significantly enhanced by the infiltration of the photonic crystal with other classes of materials, particularly highly nonlinear liquid crystals and electro-optical materials. The properties of conventional 2D PC slab waveguides were simulated by the finite difference time domain method and shown to exhibit very large refraction and dispersion, and significant tunable effects under bias when infiltrated with liquid crystal. In particular, a new superlattice photonic crystal concept is proposed and shown to exhibit up to  $\sim 50^{\circ}$  tunability in the angle of refraction when alternate liquid crystal infiltrated pixel rows were modulated from their aligned to unaligned state. This modulation corresponds to index changes from 1.5 to 2.1; it is assumed that a refractive index change of up to approximately  $\Delta n = 0.6$  can be achieved. The superlattice effect was also demonstrated to induce new switching and out-coupling effects that were strongly dependent on the direction of propagation and index modulation. These simulations demonstrate the potential of a new class of optically-active photonic crystal architectures to tune giant refraction and dispersion characteristics and to enable new switching phenomena.

### 1. Introduction

In 1987, Yablonovitch and John independently proposed the possibility of photon confinement and the suppression of spontaneous emission by the use of material that possessed a periodic dielectric contrast in three dimensions.<sup>1,2</sup> Essentially, Yablonovitch and John extended the idea of the multilayer stack to three dimensions so that the dielectric periodicity now covered three dimensions. As shown by Joannopoulos, Meade and Winn,<sup>3</sup> a photonic crystal is analogous to a semiconductor, but whereas Schrödinger's equation is used to describe the behavior of electrons in a semiconductor, Maxwell's equations are used to describe photons travelling in a photonic crystal (PC). The result is a characterization of the allowable photon frequencies in terms of an eigenvalue problem. These solutions result

in band structure diagrams, density of states plots, defect modes, as well as transmission and reflection coefficients and dispersion surface plots. In fact, many other concepts in solid-state physics also transfer over to photonic crystals such as the reciprocal lattice and Brillouin zone (BZ). The initial attention in this field was focused on creating a complete photonic band gap (PBG) and with various defects that would allow guided modes, resonances and many other unique properties, thus opening the possibility for new devices and the miniaturization of existing devices. However, another important property directly resulting from the band structure is the highly nonlinear dispersion properties near the BZ edge, which can lead to many interesting ways to control light. These properties were first demonstrated by Lin *et al.* in 1996, who reported the ability to refract EM radiation  $46.5^{\circ}$  from its original path.<sup>4</sup> This experiment was conducted at millimeter wavelengths (75– 110 GHz) using alumina rods arranged in a triangular lattice. Kosaka et al.<sup>5</sup> later demonstrated a similar effect at  $\lambda = 0.956 \ \mu m$  using an alternating Si–SiO<sub>2</sub> structure that resembled graphite and attributed the origin of their "superprism effects" to a strong modification of the dispersion surface that directly affects the group velocity rather than the phase velocity that was measured by Lin. Recently, Wu  $et \ al.^6$  reported the observation of super-prism effects in a guided mode and Baba et al.<sup>7</sup> demonstrated that a resolution of 0.4 nm can be achieved with these devices.

In 1999 Busch and John<sup>8</sup> proposed that the PBG could be tuned by infiltrating the PC with a highly nonlinear material, such as a liquid crystal (LC).<sup>9</sup> This was soon demonstrated by Yoshino *et al.*,<sup>10</sup> and Leonard *et al.*<sup>11</sup> who used the temperature dependence of the refractive index of a LC to tune the photonic band gap of a photonic crystal. For these measurements the LC was, respectively, infiltrated into a silica opal, and also a 12-micron thick Si PC with a 1.58-micron pitch. Leonard *et al.* also identified the LC mechanism as an escaped-radial alignment of the director, and showed that consequently the tunability was approximately ~60% of the full index change. In the structures modelled in this paper the aspect ratio of the LC hole diameter, *d*, to the waveguide thickness, *a*; that is d/a is ~1.5 and thus the electric field modulation of the LC should be fairly high, and probably exceeds the conditions determined by Leonard *et al.* 

The beam steering and tunability that could be obtained in a 2D PC that was infiltrated with LC was first reported by Park and Summers, who also introduced a new concept, that of a superlattice photonic crystal (SL PC).<sup>12</sup> Recently, it has also been proposed that tunable refraction effects can be achieved by etching a PC triangular lattice into a ferroelectric, although these authors did not consider the very important implication of guiding in a 2D slab.<sup>13</sup>

## 2. Homogeneous Infiltrated Photonic Crystal

In a previous paper we reported that a 2D triangular lattice exhibits very large refraction and dispersion effects.<sup>14,15</sup> In this work we extend this structure and investigate the effect of infiltrating a 2D triangular lattice with a nonlinear or



Fig. 1. Schematic of 2D PC slab, indicating the assumed alignment of the liquid crystal in the unbiased and biased state.

electro-optical material that can exhibit a very large change in refractive index when electrically or optically biased. Essentially, we have investigated the properties of LC infiltrated photonic crystals and the effect of externally biasing the structures so as to realize an increase in refractive index from  $\sim 1.5$  up to 2.1; that is a  $\Delta n = 0.6$ . These values are based on the recent reports by Wu *et al.*, who have developed new LCs with very high birefringence.<sup>16</sup> The device configuration is shown schematically in Fig. 1. It consists of a silicon slab waveguide of refractive index 3.45, in which a triangular lattice of holes is patterned into the substrate with a lattice constant of a, and hole radius, r = xa, where x typically ranges from 0.2 to 0.4. For the simulations reported, an x-value between 0.2 and 0.35 was used; the slab thickness was 0.5a, and solutions to the Maxwell's equations are obtained using the finite difference time domain (FDTD) method. The photonic band structures obtained for a triangular lattice of holes filled with LC in a 2D slab are shown in Fig. 2 for the TE-like polarization mode. This data shows the presence of a photonic band gap between the first and second bands and that there are significant variations in the photonic band structure throughout the E versus k-space. In contrast, for an isotropic medium, the energy band structure is just a single line with a slope given by the formula:

$$\omega(k) = \frac{ck}{\sqrt{\varepsilon}} \,.$$

This plot is termed the "light-line", and at any given energy the k-vectors are equal in magnitude in all directions. In a photonic crystal the E versus k relationship becomes highly anisotropic. The conditions for dispersion can then be estimated from the energy band diagram, by selecting energies for which there is a large



Fig. 2. Photonic energy band structure for a 2D triangular lattice PC structure showing the dispersion diagram obtained for a constant frequency line at a normalized frequency of 0.355.

directional variation in k-vector. The selection criteria can be deduced by observing at a single frequency: (1) the slope of the bands and (2) the relative distance from the  $\Gamma$  point of the point of intersection of the equi-frequency line with the respective band. For example, as shown in Fig. 2 at a normalized frequency of 0.355, along the  $\Gamma$ -M direction the 3rd band crosses the line near the M-point with a relatively flat slope whereas along the  $\Gamma$ -K direction it crosses the band with a larger slope and is closer to the  $\Gamma$ -point. The distance between these two points determines the basic shape and sharpness of the dispersion curve for the 3rd band, which will be star-shaped because of the triangular geometry of the PC. By computing several dispersion curves each with a slightly different energy, the field gradient at the diffraction point was determined. This identifies the direction of the Poynting vector and therefore the sign of the refraction.

To obtain the full dispersion diagram Maxwell equations were solved for a constant energy so as to find all k-values that satisfy the equations. As shown in Figs. 3(a) and 3(b) for a triangular lattice two types of dispersion curves can be obtained. A star-shaped dispersion characteristic in which the peaks align along the  $\Gamma$ -M directions and an inverted cone-shaped characteristic aligned along the  $\Gamma$ -K directions. In both figures the isotropic guiding region given by the light-line is shown: modes within this circle are not guided and will be free modes that can propagate out of the crystal.

For Fig. 3(a) the refraction properties were calculated for incident angles,  $\theta_i$ , ranging from 0° to -9°. This range is limited by the fact that (as shown in the inset) for larger angles the dispersion curve crosses the light-line circle defining the guiding condition and thus the beam can no longer propagate along the waveguide and will be out-coupled. Using the fact that the tangential component of the k-vector must



Fig. 3. (a) Dispersion curves and refraction effects obtained for the energy band structure shown in Fig. 2, for a normalized frequency of 0.355. Negative refraction vs. angle of incidence for a star-shaped dispersion curve aligned along the  $\Gamma$ -M direction. (b) Negative refraction obtained for a cone-shaped dispersion curve aligned along the  $\Gamma$ -K direction, hole radius of 0.3*a* and normalized frequency of 0.36.

be conserved at the interface between the host material and the photonic crystal the refraction angle was determined as a function of the angle of incidence. As shown the angle of refraction depends strongly on the angle of incidence, increasing rapidly to  $\sim 70^{\circ}$  for a small increase of  $0^{\circ}$  to  $-3^{\circ}$  in the incidence angle. By repeating this procedure for different bias conditions, that is for a range of LC refractive index values, for which n = 1.5, 1.7, 1.9, and 2.1, it was found that all curves exhibit the giant refraction effect, but that the dependence of the  $\theta_i$ , versus  $\theta_r$ , curves on the index change was fairly small, in the order of  $5^{\circ}$ . Thus the tunability in the angle of refraction that can be obtained with an applied bias is likewise relative small. The sign of refraction was determined from the gradient of the dispersion curves, and is negative and positive respectively, in the cases shown, i.e. in Fig. 3(a) the refracted beam is bent towards the direction of the incident beam.

As shown in the inset of Fig. 3(b), for light incident on the PC along the  $\Gamma$ -K direction the dispersion curve has an inverted shape; basically if one expands the star-shaped curve across the BZ then the equal-energy contour curves assume the shape shown in Fig. 3(b). As a consequence the dispersion curves are cone-like in shape and become symmetrical about the  $\Gamma$ -K axis. This is a direct result of the 3rd band's shape. The refraction behavior was calculated in a similar manner to the star-shaped dispersion curves and is shown in Fig. 3(b). Giant refraction effects are observed for all simulations up to an angle of 30°. As n is increased the inverted cone expands and moves inwards towards the  $\Gamma$ -point, and at some value of n will intersect the light-line. For n = 2.1 this results in all modes at small angles of incidence being out-coupled. Guided modes begin at an angle of incidence corresponding to  $\theta_i$ , ~13°, and are immediately refracted by an angle of ~47°. From the separation between these curves the maximum tunability of the angle of refraction occurs at an angle of incidence of 13° and is estimated to be approximately 7°.

Because of the limited tunability range predicted for these devices, the potential of new material structures to provide enhanced effects and greater functionalities were investigated, as described below.

### 3. Photonic Crystal Superlattices

In this device an additional periodicity in the z-direction is created by alternative biasing of the LC filled holes as shown in Fig. 4. This allows the creation of a large change in refractive behavior with only a modest change in the refractive index of the crystal. The bias can be either electrical as shown, or optical, where a modulation in the refractive index is achieved by depositing opaque covers over the rows (light circles) that are not to be modulated. Illuminating the structure from the top creates the desired effect.

As shown in Fig. 4 the conventional triangular lattice has three equivalent  $\Gamma$ -M directions:  $\Gamma$ -M along the z-axis, and the  $\Gamma$ -M' and  $\Gamma$ -M" directions, respectively, that are at 60° to each other and perpendicular to any of the rows that connect the side of a triangle. Similarly, there are three equivalent  $\Gamma$ -K directions parallel to each side of the triangular lattice,  $\Gamma$ -K,  $\Gamma$ -K', and  $\Gamma$ -K", respectively. The bias shown in Fig. 4 is effectively along the  $\Gamma$ -K direction of the conventional triangular lattice.



Fig. 4. Superlattice photonic crystal structure obtained by biasing alternate rows of a liquid crystal infiltrated photonic crystal.



Fig. 5. Real space photonic crystal lattice, with imposed superlattice behavior and the subsequent transformation into reciprocal lattice space.

When unbiased, the real space lattice is the regular triangular lattice with 6-fold rotational symmetry as shown in Fig. 5(a), where  $a_2$  is the lattice parameter. This transforms into the reciprocal lattice that is also a triangular lattice but rotated by 30° with respect to the orientation of the real space lattice, shown in Fig. 5(b). However, the imposition of the SL along the z-direction, shown as alternate rows of dark and light circles, reduces the symmetry of the real space lattice such that the symmetry is now described by a rectangular lattice, shown by vectors  $a_1$  and  $a_2$  along the z- and y-directions, respectively. Thus, a larger unit cell must be used to describe this perturbation, in which there are two atoms per unit cell.

As shown in Fig. 5(b), the consequence of the superlattice is to generate a new reciprocal lattice, which is rectangular in shape and falls within the hexagonal reciprocal lattice of the original lattice. Basically the effect of the superlattice is to fold the original BZ for the triangular lattice into the rectangular reciprocal lattice of the superlattice structure. The effect of this reduced BZ is to make some of the k-vector equivalent. Now, only four of the original M-points remain equivalent (those connected by  $\Gamma$ -M' and  $\Gamma$ -M''). The two M-points connected along the  $\Gamma$ -M direction are folded in towards the center  $\Gamma$ -point. For the K-points the effect of the superlattice is to fold all of the K-points, so that only two equivalent points remain. Both of which are along the  $\Gamma$ -K' axis and equidistant from the center  $\Gamma$ -point.

The impact of this on the dispersion curves at a constant frequency is shown in Fig. 6. Figure 6(a) shows the effect of the SL on a LC-infiltrated PC with n = 1.5, but with an infinitesimally small index modulation. As shown the BZ folding transforms the modes along the  $\Gamma$ -M points into the rectagular lattice, such that they now become unguided and will be out-coupled from the 2D slab. The modes centered at the four equivalent M-points are also folded into the rectangular BZ and become asymmetrical about the corners of the zone. Figure 6(b) shows the effect that will occur when the SL is activated by applying a bias such that a difference of  $\Delta n = 0.1$  in refractive index is introduced between alternate rows.



Fig. 6. Effect of the superlattice photonic crystal structure on the dispersion curves for a range of  $\Delta n$  values: (a) for an infinitely small index modulation, (b) for  $\Delta n = 0.1$ , (c) for  $\Delta n = 0.3$ .

Quite different results were obtained as a consequence of the change in both the refractive index and the periodicity. The refraction and propagation properties are now observed to depend strongly on the direction of the incident light. For light incident along  $\Gamma$ -X', perpendicular to the electrodes the dispersion is not significantly affected. However, BZ-folding transforms what were guided modes in the slab waveguide into radiation modes that can couple light out of the waveguide. Additionally, for light propagation along the  $\Gamma$ -K or  $\Gamma$ -X direction (parallel to the electrodes) the unbiased PC exhibits a stop band so that no modes can be supported by the waveguide. However, switching on the index modulation to activate the superlattice PC is observed to create an additional mode around the X-points

along which light can propagate. The shape of the dispersion curve is such that light can propagate with modest refraction or is reflected. As the index is increased, such that  $\Delta n = 0.3$ , Fig. 6(c) shows that the dispersion curves change significantly: mode 1 moves slightly inward, mode 2 becomes separated significantly from the  $\Gamma$ -point, and mode 3 disappears. Thus, the refraction and switching behavior are affected significantly.

Figure 6(b) shows that the superlattice has three modes along  $\Gamma$ -M, but that only two are guided modes that lie completely outside the cut-off circle. Basically, when folded out the outermost mode (mode 1) can be shown to have a flattened elliptical shape about the M-point as shown in Fig. 6(b). This arises because the mode must be continuous as it crosses the BZ boundary. This flattening consequently results in two localized regions along the dispersion curve that have a much sharper curvature than the rest of the dispersion surface. The first of these regions occurs in a clockwise direction with respect to the  $\Gamma$ -M direction after which the curvature is similar to that of the triangular lattice. The refractive behavior resulting from these dispersion curves is shown in Fig. 7. Thus, proceeding clockwise from the  $\Gamma$ -M direction, for mode 1 the angle of refraction increases from 5° to 30° as the angle of incidence,  $\theta_i$ , is increased from zero to 7° (Fig. 7(a)). The behavior of this mode also has a similar dependence on  $\Delta n$ .

For light incident from a direction counter-clockwise from the  $\Gamma$ -M direction a far more complex behavior is predicted. Initially, the dispersion curve is rather flat, but as the angle of incidence is increased, such that the tangential component of the k-vector approaches the localized region of sharper curvature on the dispersion surface, the angle of refraction increases very rapidly with  $\theta_i$ . This behavior is



Fig. 7. Angle of refraction as a function of incident angle with respect to the  $\Gamma$ -M normal direction for a SL PC structure at a normalized frequency of 0.3545 (a) mode 1 and (b) mode 2.

observed in the dependence of  $\theta_r$  on  $\theta_i$ . For small angles of incidence, the dependence of  $\theta_r$  on  $\theta_i$  is small as the curvature of the dispersion surface is very shallow in this region. However, when the localized regions of high curvature are scanned, the angle of refraction becomes strongly dependent on the angle of incidence. For  $\Delta n = 0.3$ the angle of refraction increases from 7 to 60 degrees as the angle of incidence is advanced from 20° to 30°. In fact the same behavior is predicted for all values of  $\Delta n$ , but the regions of giant refraction occur at smaller angles of incidence. These effects are expected to have very important applications for beam steering and rastering. Most importantly, Fig. 7(a) shows that at a constant angle of incidence of  $\simeq 20^\circ$  the refracted beam can be electrically scanned through an angle of  $\sim 50^\circ$ , by applying a bias such that the magnitude of  $\Delta n$  in the LC is changed by 0.5. It should also be noted that the regions, where the angle of refraction is independent of the incident angle, can also have important technological applications, as this effect could be used to collimate several beams that are incident onto the PC at different angles.

For mode 2, the effect of increasing the modulation of the SL has little effect on the curvature of the disperion curve, but has the effect of progressively moving the mode further away from the  $\Gamma$ -point towards the longest side of the BZ. As such this mode lies on the clockwise side of the  $\Gamma$ -M direction for all values of  $\Delta n > 0.2$ . This results in the dependence of the refraction angle on incidence angle shown in Fig. 7(b). Consequently, the refraction properties are limited by the cut-off due to the circular light cone on one side of the  $\Gamma$ -M direction and by the edge of the BZ on the other side. Between these two limits the refraction behaves very linearly and changes in  $\theta_r$  of up to 8° can be achieved by biasing.

### 4. Summary

Investigations of a 2D PC slab Si waveguide with a regular triangular lattice that was infiltrated with LC demonstrates that these structures exhibit large angles of refraction, but that there is little tunability when the crystal was biased so as to increase the index in the holes of the waveguide. For a 15% change in index the beam steering range is estimated to be  $\sim 10^{\circ}$ . To address this limitation a new superlattice configuration was proposed as a means of introducing an additional refractive index modulation. The effect of this structure was to create new allowed modes of propagation within the waveguide and to drastically enhance the tunability and control that can be achieved over the optical properties. This new functionality improved beam steering capability, by over 50°. Highly directionally-dependent switching and out-coupling effects were also found. The combination of these techniques provides the potential to create a new class of optically-active photonic crystal architectures with the ability to tune the dispersion and refraction characteristics and offers to dramatically extend the application of photonic crystals into new types of electro-optic and nonlinear devices and systems.

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