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# Electrically tuned phase transition and band structure in a liquid-crystal-infilled photonic crystal

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We studied a nematic liquid crystal (LC) cylinder under the action of an axial electric field $\mathbf{E}_0$. Elaborate modeling of the free energy leads to the conclusion that the configuration of the molecules is "escaped radial" for low $E_0$; a phase transition, however, occurs for a critical value $E_c$, the configuration becoming axial for $E_0 > E_c$. From these results, the position-dependent dielectric tensor is determined and the photonic band (PB) structure is calculated for a photonic crystal of LC cylinders. It is shown that by varying $E_0$ a PB gap can be fully tuned from open to closed. Also, switching to a supercritical field can give rise to interesting polarization and directional effects in the propagation of light.

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Photonic crystals (PCs)—spatially periodic, composite materials that can exhibit photonic band (PB) gaps for light propagation—have reached a mature state of development, with their optical properties well understood and with many realized and potential applications [1]. Most of this research deals with PCs whose characteristics are fixed, that is, once they have been fabricated there is no possibility to alter their optical response. A recent trend, however, concerns tunable or active PCs; by this we imply that, by means of some external agent, it becomes feasible to change the optical properties of the PC continuously and reversibly. This could lead to tunable optical waveguides, switches, limiters, and polarizers; to reconfigurable optical networks; and to electro-optic interconnects in microelectronics.

The tuning or switching of PCs has been proposed or achieved by producing structural changes, by the incorporation of a ferromagnetic material, by varying the density of the plasma of free electrons in a semiconductor constituent, by taking advantage of optical nonlinearities caused by intense laser illumination, and by infilling the PC with a liquid crystal (LC). Some 50 papers have been published on the subject, recently explored at a specialized conference [2]. In particular, LCs are well-established electro-optic materials that can be tuned by means of pressure, heat, and applied electric or magnetic field. Their incorporation within a PC is of particular interest because of the possibility of selectively tuning PB gaps, as reviewed recently [3].

In 1999, Bush and John [4] pointed out that, when a nematic LC is infiltrated into the void regions of an inverse opal PC, the resulting composite exhibits a completely tunable PB gap. In their calculation, this is achieved by an electric field, which rotates the axes of the LC molecules relative to the opal backbone. This, however, requires external fields strong enough to overcome the Van der Waals forces on the molecules. Moreover, the rotation of the electric field is very cumbersome experimentally. Further, these PCs are disadvantageous because they have a high density of defects and only pseudogaps restricted to the [111] direction. Finally, the anchoring problem in opal PCs is extremely complicated [5], thus hindering theoretical analysis. For all these reasons, the LC tuning of the PCs has not lived up to the blueprint and promise originally outlined. More than anything else, theory has lagged much behind experiment; in fact, there is no first principles theory that predicts the response of a LC-infilled three-dimensional (3D) or two-dimensional (2D) PC to an applied field. In this paper, we present just such a theory for 2D PCs of hollow cylinders, infilled with a nematic LC. We argue that such PCs are advantageous for tuning by modest electric fields that are parallel to the cylinders. This is so because of their relative simplicity and high quality of fabrication; because typically large material contrasts lead to large PB gaps in all the in-plane directions; and because the theory of a dielectric response of a LC cylinder is a manageable problem, that can lead to convergence with experimental studies. Leonard*et al.* [6] have already infilled a 2D macroporous Si PC with a nematic LC and showed that temperature tuning can be accomplished by provoking a transition of the LC from the nematic to the isotropic phase. The same type of transition was employed to tune the transmission peak of a wave guided by a III-V semiconductor PC with a missing row of cylinders [7]. The selective tuning of light propagation in a *Y*-shaped, LC-infilled PC waveguide was also theoretically studied [8]. Further, very recently, electric tuning of a 2D PC laser was accomplished [9].

We study the detailed nature of the interaction of the nematic LC with the cylinder wall and the applied field. Minimizing the free energy, we show that, for a critical value of the field, the molecules undergo a second-order configurational phase transition. We determine the dielectric tensor at every point within a LC cylinder, leading to the PB structure, which exhibits polarization-dependent tuning and switching behaviors.

First, we focus on a single, infinite, circular cylinder of a nematic LC. In order to determine the molecular or "director" orientations $\hat{\mathbf{n}}(\mathbf{r})$ $[|\hat{\mathbf{n}}(\mathbf{r})|=1]$ at a point, we consider the Helmholtz free energy. This has an elastic part or Franck energy (corresponding to the Van der Waals forces) of the form $(1/2)K_{ijkl}(\nabla_i n_j)(\nabla_k n_l)$, a surface "anchoring" part, and an electromagnetic part $(-1/2)\mathbf{D}_0 \cdot \mathbf{E}_0$, with the wave field $\mathbf{E}$

 

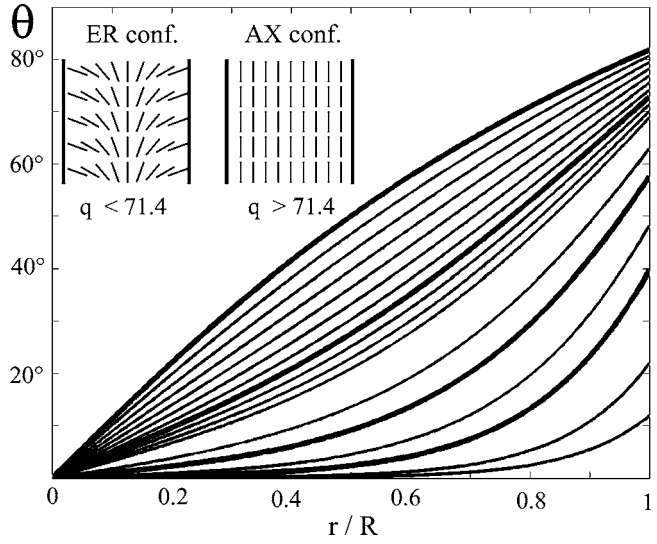


FIG. 1. The angle $\theta(r/R)$ between the nematic director $\hat{\mathbf{n}}(r)$ and the cylinder axis $\hat{\mathbf{z}}$, as the function of the normalized radial distance inside a liquid crystal cylinder. The curves correspond to the field parameter $q=\varepsilon_a R^2 \mathbf{E}_0^2/K_{11}$, taking the values (from above) **0**, 1, 2, 3, 4, 5, 6, 7, 8, **9**, 11, 15, **20**, 30, **40**, 60, 70 (the curves for $q=0,9,20,40$ are drawn in heavy lines because they correspond to four cases considered in Fig. 3). For $q\simeq 71.4$, a phase transition occurs from the escaped radial to the axial configuration shown in the insets.

neglected in comparison to the static field $\mathbf{E}_0$ (linear approximation). With $\mathbf{E}_0 \| \hat{\mathbf{z}}$ (cylinder direction) the free energy is (Refs. [10,11])

$$F = \frac{1}{2}\Bigg\{ \int_V dV[K_{11}(\boldsymbol{\nabla}\cdot\hat{\mathbf{n}})^2 + K_{22}(\hat{\mathbf{n}}\cdot\boldsymbol{\nabla}\times\hat{\mathbf{n}})^2 + K_{33}(\hat{\mathbf{n}}\times\boldsymbol{\nabla}\times\hat{\mathbf{n}})^2 - K_{24}\boldsymbol{\nabla}\cdot(\hat{\mathbf{n}}\boldsymbol{\nabla}\cdot\hat{\mathbf{n}} + \hat{\mathbf{n}}\times\boldsymbol{\nabla}\times\hat{\mathbf{n}})] + \int_S dS W_\theta \sin^2\theta(r) - \int_V dV(\varepsilon_o + \varepsilon_a n_z^2)E_0^2 \Bigg\}. \quad (1)$$

The elastic moduli $K_{11}$, $K_{22}$, $K_{33}$, and $K_{24}$ describe, respectively, transverse bending ("splay"), torsion ("twist"), longitudinal bending ("bend"), and surface interaction. $W_\theta$ is the strength of anchoring of the molecules at the walls, and $\theta(r)$=angle $[\hat{\mathbf{n}}(r),\hat{\mathbf{z}}]$. In the last term, $\varepsilon_o$ and $\varepsilon_a$ are the ordinary dielectric constant and the "dielectric anisotropy" ($\varepsilon_a=\varepsilon_e-\varepsilon_o$) of the LC. Assuming axial symmetry, the director is $\hat{\mathbf{n}}=\sin\theta(\hat{\mathbf{x}}\cos\varphi+\hat{\mathbf{y}}\sin\varphi)+\hat{\mathbf{z}}\cos\theta$. Integrating over $\varphi$, the free energy per unit length is obtained. The *stationary* orientational configuration $\theta(r)$ is determined by minimizing the free energy. This leads to the following Euler-Lagrange equation (with primes denoting differentiation with respect to the argument $x=r/R$, $R$ is the cylinder radius) [11]:

$$[\cos^2\theta(x) + \eta\sin^2\theta(x)][x^2\theta''(x) + x\theta'(x)] + \tfrac{1}{2}\sin 2\theta(x)\{(\eta-1)x^2[\theta'(x)]^2 - qx^2 - 1\} = 0, \quad (2a)$$

with the condition $\theta(0)=0$ on the axis and the boundary condition at the surface ($x=1$)

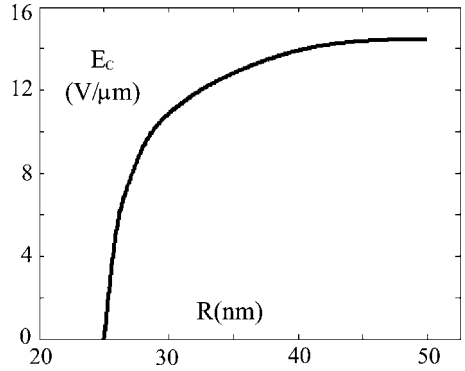


FIG. 2. The critical applied electric field for transition from the escaped radial to the axial configuration of the nematic liquid crystal cylinder, as a function of the cylinder radius.

$$\theta'(1) = \tfrac{1}{2}\sigma\sin 2\theta(1)/[\cos^2\theta(1) + \eta\sin^2\theta(1)]. \quad (2b)$$

$\eta=K_{33}/K_{11}$, $\sigma=W_\theta R/K_{11}+K_{24}/K_{11}-1$, and $q$ is the "field parameter"

$$q = \varepsilon_a R^2 E_0^2/K_{11}, \quad (3)$$

representing the ratio of the electric and elastic energies. For $q\ll 1$ the influence of the applied field is weak, while for $q\gg 1$ the field essentially overcomes the Van der Waals forces.

Equation (2) has two simple exact solutions, namely, $\theta=\pi/2$ and $\theta=0$. The first possibility corresponds to the "planar radial" (PR) configuration with $\hat{\mathbf{n}}(\mathbf{r})\perp\hat{\mathbf{z}}$; the second is the "axial" (AX) configuration with $\hat{\mathbf{n}}=\hat{\mathbf{z}}$. A third solution is the "escaped radial" (ER) configuration, with the directors fanning out from the cylinder axis to its wall, Fig. 1, left inset. We have selected the nematic LC "5CB" for our numerical study; the ordinary permittivity and anisotropy are $\varepsilon_o=7$, $\varepsilon_a=11.5$ for low frequencies and $\varepsilon_o=2.403$, $\varepsilon_a=0.605$ for optical frequencies, all in units of the vacuum permittivity. Note that the former values are used in Eqs. (1)–(5) and the latter in Eqs. (6) and (7). Other parameters are $K_{11}=1.2\times10^{-11}$ N$=K_{24}$, $\eta=1.316$, $W_\theta/K_{11}=40$ $\mu$m$^{-1}$; hence $\sigma=40R$ [$\mu$m] [12]. The solutions for $\theta(r)$ have been found by the shooting method [13], and are shown in Fig. 1 for $R=0.2$ $\mu$m and a series of values of the field parameter $q$, Eq. (3). It is seen that, on the cylinder wall ($r/R=1$), in the absence of the field ($q=0$), the director does not deviate much from the perpendicular direction; it becomes more and more aligned with the cylinder as the field increases.

The ER configuration, in fact, is realized for relatively large $R$ and $\mathbf{E}_0=0$ [14]. Is it possible, however, that a phase transition occurs for a different configuration for a sufficiently strong field? The "planar polar" and the PR configurations are not plausible and, indeed, if we set $\theta(x)=\pi/2$ in Eq. (2), we find that $F_{\mathrm{PR}}(q)>F_{\mathrm{ER}}(q)$. On the other hand, if we set $\theta(x)=0$ in Eq. (2), we get

$$F_{\mathrm{AX}}(q) = \pi K_{11}(W_\theta R/K_{11} - \varepsilon_e q/2\varepsilon_a), \quad (4)$$

and the AX configuration becomes more stable than the ER provided that $F_{\mathrm{AX}}(q)<F_{\mathrm{ER}}(q)$. This can occur for suffi-

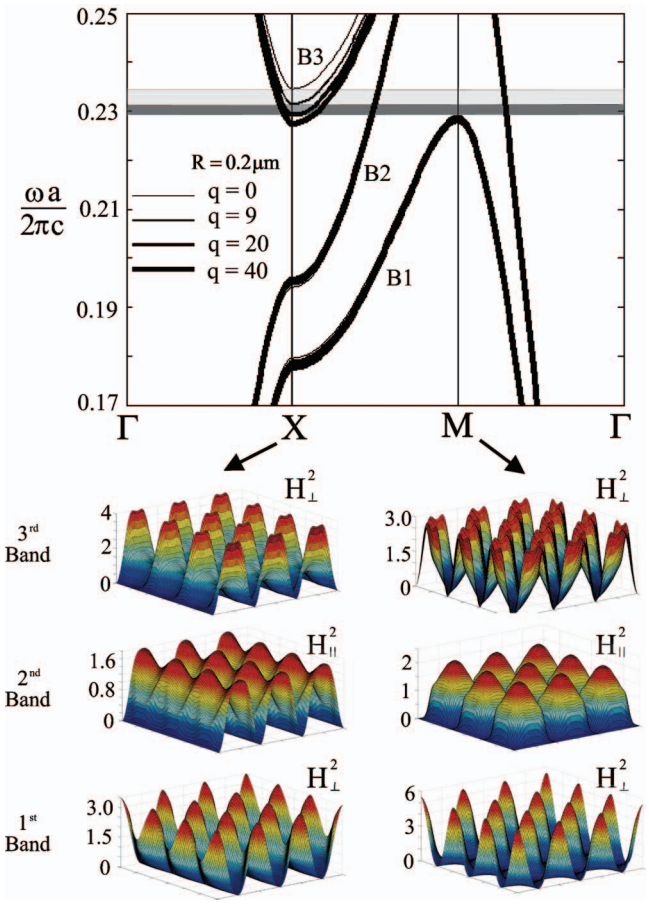


FIG. 3. (Color) Top: Band structure for a square lattice of LC cylinders in Si. The first three bands are plotted for four values of the field parameter $q$. (The corresponding $\theta(r)$ curves in Fig. 1 are rendered thicker.) Bands 1 and 3 (2) have their $\mathbf{E}(\mathbf{H})$ field very nearly parallel to the cylinders, as can be understood from the magnetic field eigenvectors (below). These are shown for the first three bands at the $X$ and $M$ points of the Brillouin zone. For the first and third bands, $H_{\perp}^2(\mathbf{r})$ is shown; $H_{\parallel}^2(\mathbf{r})$ is very small, with the average value $\langle H_{\parallel}^2\rangle < 3\times 10^{-3}\langle H_{\perp}^2\rangle$ in all cases plotted. For the second band $H_{\parallel}^2(\mathbf{r})$ is exhibited and $H_{\perp}^2(\mathbf{r})$ is extremely small, with $\langle H_{\perp}^2\rangle < 3\times 10^{-5}\langle H_{\parallel}^2\rangle$. Note that there is a completely tunable gap for $E$ polarization.

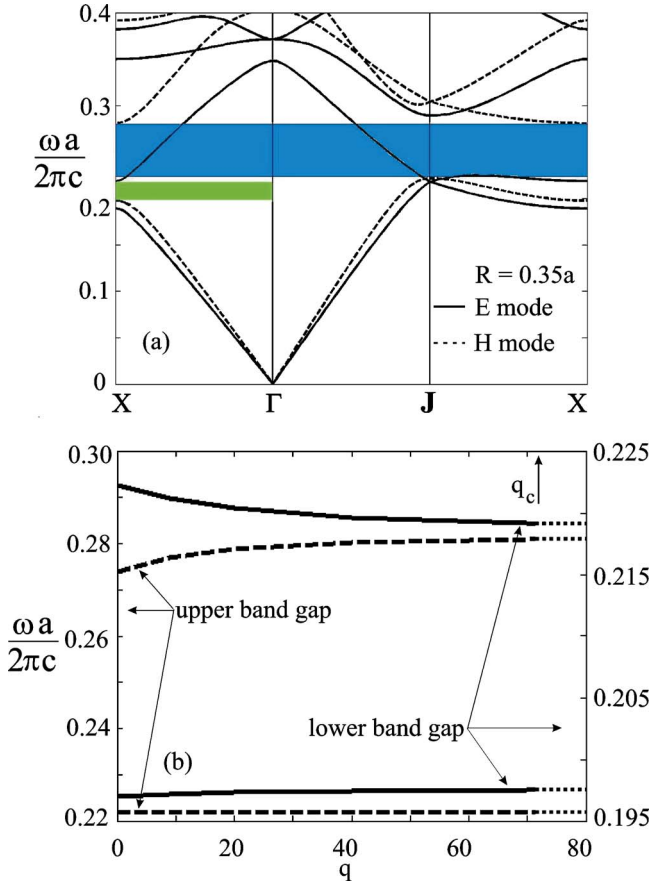


FIG. 4. (Color online) (a) Band structure for supercritical fields ($q > 71.4$), that is, axial configuration of the liquid crystal (triangular lattice). Note a complete (partial) band gap for $H$-polarized (unpolarized) light. (b) The edges of the two forbidden (shaded) bands in (a) as a function of the field parameter. A phase transition occurs from the ER to the AX configuration at $q = 71.4$.

ciently large fields, such that $q > q_c$, where the critical value $q_c$ is given by

$$F_{\mathrm{ER}}(q_c) = \pi W_{\theta} R - \pi K_{11}\varepsilon_e q_c^2/2\varepsilon_a. \tag{5}$$

The corresponding critical electric field is plotted in Fig. 2 as a function of the cylinder radius. We see that, with the exception of extremely small radii ($R < 50$ nm), the critical field is $E_c \simeq 14$ V/$\mu$m. For $R = 0.2$ $\mu$m this gives $q_c = 71.4$, from which it follows that, in Fig. 1, $\theta = 0$ for $q > 71.4$.

Now that we have determined $\theta(r)$ for all $\mathbf{E}_0$, we proceed to calculate the elements of the dielectric tensor $\varepsilon_{ij}(r)$ of the LC cylinder. Of course, in the proper system of the LC at a point $\mathbf{r}$, $\varepsilon_{ij}$ has the uniaxial form, given in terms of $\varepsilon_o$ and $\varepsilon_e$. Transforming to the "laboratory" system,

$$\varepsilon_{ij}(r) = \varepsilon_o \delta_{ij} + \varepsilon_a n_i(r) n_j(r), \quad (i,j = x,y,z) \tag{6}$$

with $\hat{\mathbf{n}}(\mathbf{r})$ given after Eq. (1). Clearly, the problem at hand is both anisotropic and inhomogeneous. The host material is chosen to be Si with permittivity $\varepsilon_{\mathrm{Si}} = 11.7$. The PB structure is obtained from the wave equation for the magnetic field,

$$\boldsymbol{\nabla} \times \{\overleftrightarrow{\boldsymbol{\varepsilon}}^{-1}(\mathbf{r}) \cdot [\boldsymbol{\nabla} \times \mathbf{H}(\mathbf{r})]\} = (\omega/c)^2 \mathbf{H}(\mathbf{r}) \tag{7}$$

where the dyadic $\overleftrightarrow{\boldsymbol{\varepsilon}}^{-1}(\mathbf{r})$ is found from the inversion of $\varepsilon_{ij}(\mathbf{r})$ for $\mathbf{r}$ within a cylinder. $\mathbf{H}(\mathbf{r})$ must be a superposition of plane waves with wave vectors $\mathbf{k}+\mathbf{G}$, where $\mathbf{k}$ and $\mathbf{G}$ are the Bloch and reciprocal-lattice vectors. It has two components that are perpendicular to $\mathbf{k}+\mathbf{G}$; these are coupled because of the anisotropy. Hence, despite of the 2D periodicity, *strictly speaking*, there are no modes with their electric or magnetic field polarized parallel to the cylinders.

The first three bands of a typical band structure (with $\omega$ normalized by the PC period a) are shown in Fig. 3 (top) for four values of the field parameter. The first two bands are rather insensitive to $\mathbf{E}_0$, and it is band 3 that is responsible for most of the tuning. Below in Fig. 3 the eigenvectors—actually the square of the perpendicular (for bands 1 and 3)

or parallel to $\hat{\mathbf{z}}$ (for band 2) component of $\mathbf{H}_{\mathbf{k}}(\mathbf{r})$—are plotted in nine unit cells, for $\mathbf{k}$ corresponding to the $X$ and $M$ points of the Brillouin zone. The important conclusion is that $H_{\perp}^2 \gg H_{\parallel}^2$ for the first and third bands, while the reverse is true for the second band. Therefore, we may regard the modes corresponding to the first and third bands as *nearly* $E$-polarized ($\mathbf{E} \| \hat{\mathbf{z}}$), while those corresponding to the second band are *nearly* $H$-polarized ($\mathbf{H} \| \hat{\mathbf{z}}$). Now, it becomes apparent that *there is a completely tunable PB gap for E modes between the first and third bands*: in the absence of an applied field ($q=0$) and for small fields ($q=9$) a wave incident at the PC with $\mathbf{k} \perp \hat{\mathbf{z}}$ and $\mathbf{E} \| \hat{\mathbf{z}}$ will be completely reflected for $\omega$ within the gap; for $q=20$ the gap closes; and for $q=40$ (large applied field) the bands overlap, thus allowing propagation.

While Fig. 3 concerns *tuning* (by subcritical fields), Fig. 4 is an example of *switching*—from the field "off" to a supercritical value—taking advantage of the transition from the ER to the AX configuration. Figure 4(a) shows a wide, complete PB gap for supercritical fields with (now strictly) $H$ polarization, and there is a smaller gap for propagation limited to the $\Gamma X$ direction, however, for any polarization of the incident wave. In Fig. 4(b), we see the approach to criticality of the edges of the two aforementioned band gaps; for $q > q_c = 71.4$ these band edges do not shift anymore and coincide with the corresponding values in Fig. 4(a). As an example of switching, if the PC is illuminated by the *unpolarized* light of the frequency $\omega a / 2\pi c = 0.276$, for $\mathbf{E}_0 = 0$ both $E$ and $H$ components will be transmitted. On the other hand, for $\mathbf{E}_0 > E_c$, only the $E$-polarized component is transmitted.

Quite independently of the PCs, this paper established the existence of a phase transition—from the ER to the AX configuration—within a single LC cylinder, reached for a critical value of the applied field $\mathbf{E}_0$. This behavior would surely be interesting to investigate for other LCs, both theoretically and experimentally. Our calculations also demonstrated that both tuning and switching of LC-infilled PCs is feasible for a system that is much simpler than opal PCs. These ideas could contribute in a significant way to "the aim to monolithically integrate tunable properties with other optoelectronic components, like lasers, waveguides and detectors" [3].

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