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Author(s)	Yoshida, Hiroyuki; Ozaki, Ryotaro; Yoshino, Katsumi et al.
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Modulation of the Photonic Band by Introduction of Phase Defects in Chiral Liquid Crystals

Hiroyuki Yoshida[1], Ryotaro Ozaki[1], Katsumi Yoshino[1,2], Masanori Ozaki[1]
[1]*Department of Electronic Engineering, Faculty of Engineering, Osaka University*
2-1 Yamada-oka, Suita, Osaka 565-0871, Japan
email: hyoshida@ele.eng.osaka-u.ac.jp
[2]*Center for University-Industry Cooperation, Shimane University, Matsue, Shimane 690-0816 Japan*

INTRODUCTION

Photonic band-gap materials have periodic structures with a periodicity of the order of wavelength of light and have attracted great interest from both practical and scientific perspectives since their first proposal by Yablonovitch [1] and John [2]. Bragg reflection of photons occurring at the interface of each layer leads to the formation of the photonic band-gap (PBG) in which propagation of light with certain wavelengths is prohibited. On the other hand, upon introduction of a defect in PBG materials, light is known to localize at the defect sites. Depending on their structure and in how many different directions the PBG is observed, one-dimensional, two-dimensional and three-dimensional photonic band-gap materials are realized. While higher-order PBG materials open ways to perfect optical trapping and fascinating applications such as lossless waveguides and thresholdless lasers, interesting phenomena and applications have been reported even in one-dimensional PBG materials, such as optical limiting [3] and band-edge lasing [4].

For the fabrication of PBG materials, semi-conductor processing techniques, which have shown vast improvement over the last several years are usually used. While semi-conductor materials have been widely studied for PBG material usage, much attention has been poured also on cholesteric liquid crystals (ChLCs), which have organic, self-organized periodic structures. As shown in Fig. 1 (a), ChLC is a kind of liquid crystals (LCs) in which their director vector rotates either clockwise or anti-clockwise with a certain pitch that arises from the *helical twisting power* (HTP) of its chirality. LCs act as an anisotropic material with a difference in the extraordinary refractive index n_e and ordinary refractive index n_o when their director vector is pointed in towards a certain direction; for the ChLC, the birefringence the helical periodicity give rise to the PBG which extends from the wavelength region $n_o p \sim n_e p$. Because of the helical periodicity, however, the PBG is exhibited only for the circularly polarized light with the same handedness as the helix sense of the material. While characteristics of typical one-dimensional PBG materials are observed in ChLCs, advantages of LC molecules result are seen in tunable lasers utilizing the sensitivity of the helix pitch to the electric field [5,6] and free-standing film type ChLC lasers prepared by photo-polymerization [7].

ChLCs are characteristic also in that a different kind of defect can be introduced due to their helical structure. Namely, modulations in the phase or periodicity can be realized due to the chiral, sinusoidal periodicity of the refractive index. Kopp *et al.* [8] theoretically proposed that introducing a twist defect where the director vector is discontinuous would lead to realization of a localized state at the twist defect site, and experimental reports of lasing from such defect

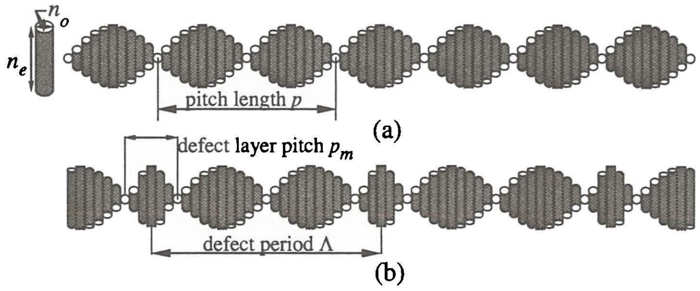

FIG 1. (a) A schematic illustration of a left-handed cholesteric liquid crystal with pitch p. (b) A schematic illustration of the system under consideration where multiple defects with a different pitch length is introduced periodically throughout the medium.

modes have been presented by Ozaki *et al.* [9]. The phase of the sinusoidal refractive index is made discontinuous in this case, while a defect mode arising from the modulation in the HTP, which corresponds to the frequency has been proposed by Matsui *et al.* [10]. Both of these defects are characteristic of the ChLC, and would not be realized in conventional PCs where the dielectric constant changes stepwise.

The modulation in the HTP, or frequency discussed here is characteristic in that the pitch modulation can be introduced to a region smaller than the initial pitch of the structure. Furthermore, it does not have to be limited to only a certain region in the ChLC, but can be distributed throughout the medium as shown in Fig. 1(b). In this study, we investigated the effect of introducing pitch modulations into a region smaller than the initial pitch of the ChLC medium. We then modeled a ChLC layer with periodic multiple defects with HTP modulation, and performed theoretical calculations of the transmission spectrum. We have employed the transfer matrix method and finite difference time domain simulation to investigate the transmission spectrum and the electromagnetic field distribution in the disordered ChLC layer. While Matsui *et al.* assumed a Gaussian distribution for pitch modulation, we assumed a stepwise change in the HTP. This assumption makes the analysis simpler, yet still does not lose the essence of defect modes arising from the pitch length discontinuity.

NUMERICAL ANALYSES

Since ChLCs have a refractive index varying along one direction, the transfer matrix method (TMM) [11] can be employed for quantitative analysis of their optical characteristics. Assuming the helical axis of the ChLC to be along the *z*-direction, light propagating along the helical axis is formulated by $d\mathbf{\Psi}(z) / dz = (i\omega/c) \times \mathbf{D}(z)\mathbf{\Psi}(z)$, where $\mathbf{D}$ is the derivative propagation matrix, and $\mathbf{\Psi}(z) = [E_x, H_y, E_y, H_x]^T$. Solving this equation numerically gives information on the transmittance of the medium for light incidence with different polarizations.

The parameters used in this study were as follows: the left-handed ChLC modeled for analysis had initial pitch length $p_0 = 400$ [nm], and the ordinary and extraordinary refractive indices of $n_o = 1.53$ and $n_e = 1.78$ respectively. This is the value for the NLC mixture E44 (Merck), which is a common ingredient in ChLCs. The ChLC was sandwiched by glass substrates with $n_{glass} = 1.5$ and the length of the ChLC material was L = 5300 [nm]. The helical twisting power (HTP) of ChLCs is defined as $q_{HTP} = 2\pi/p$ [rad/nm] using the helix pitch p. The ChLC used in this calculation has the initial value of $q_0 = 2\pi/400$ [rad/nm]. From this definition of the HTP we view each unit length of the ChLC to possess a rotary power to twist the LC director vector. By some means of an external field, this HTP would be altered with respect to the initial HTP, leading to a shorter or longer pitch. By introducing the HTP modulation factor $\alpha = (q_m - q_0) / q_0 = \Delta q / q_0$, the modulated HTP of the ChLC can be expressed as $q_m(z) = q_0(1+\alpha)$. We considered a defect layer with a shortened pitch length by HTP modulation factor $\alpha = 0.3$. The width was varied from $w_{Defect} = 500$ nm to 100 nm, which varies from $w_{Defect} / p_0 = 1.25 \sim 0.25$. Multiple defect layers were introduced in the structure, each layer separate equidistantly from its neighboring defect layers. The distance between the defect layers were varied from $\Lambda_{defect} = 1000$ nm to 400 nm and the effect on the transmission spectrum was observed. In all cases, left circularly polarized (LCP) light was assumed for incidence, because the left-handed ChLC only exhibits the PBG for LCP light.

Finite difference time domain (FDTD) method is a numerical solution to the Maxwell equations performed by converting the differentiations to simple differences by $\partial E/\partial z \rightarrow (E^j(z+1)-E^j(z))/dz$, $\partial E/\partial t \rightarrow (E^{j+1}(z)-E^j(z))/dt$. FDTD calculations allow time-resolved analyses on the electromagnetic field (EMF) distribution through a dielectric medium, and provide insight on how the EMF behaves in the structure. FDTD calculations were performed for wavelengths λ =

662 nm, 672 nm and 678 nm in the case where three defect layers ($\alpha = 0.3$, $w_{Defect} = 300$ nm) were introduced, each separated by $\Lambda_{Defect} = 1700$ nm.

RESULTS AND DISCUSSION

Figure 2 (b) shows the defect mode due to a single defect layer with the modulated HTP given by $q_m(z) = 2\pi/400(1\pm0.3)$ for different defect layer length w_{Defect}, as shown in Fig. 2(a). As w_{Defect} is increased, the defect mode shows a blue-shift for the pitch-shortening defect, whereas a red-shift is observed for elongation defects. The shift of the defect mode corresponds to the fact that the PBG of ChLCs are given by $\Delta n \times p$, indicating that a smaller pitch accounts for a PBG in the shorter wavelength region, and vice versa.

Figure 3 shows the transmission spectra of the case where multiple defect layers were introduced almost evenly in the 5.3 μm long ChLC medium, with $\Lambda_{Defect} = 1700$ nm. When multiple defects are introduced in the ChLC, a transmission band appears in the PBG of the ChLC. As w_{Defect} is increased, the transmission band exhibited a shift similar to that observed in the case where a single defect was introduced. In fact, the position of the central wavelength of the transmission band corresponds to that of the defect mode wavelength for the case where single defects were introduced. The fact that the defect mode seems to "split" is analogous to the tight-binding model in quantum physics; in quantum physics the wave function of electrons couple with their neighboring wave functions, leading to a formation of a band. The EMF distribution for the case where $w_{Defect} = 300$ nm is shown in Fig. 4. At each of the peak wavelengths in the transmission band (indicated by arrows in Fig. 3), the EMF is seen to localize at the defect sites and seen to couple. A tunable photonic transmission band is predicted by introduction of multiple HTP defect layers.

The inter-defect length was decreased to investigate the effect of introducing frequent, thin defect layers in the ChLC. The width of the defect layer was $w_{Defect} = 150$ nm, which is less than $p_0/2$ or $p_m/2$ (= 200 nm and 150 nm respectively). Figure 5 shows the transmission spectrum of the ChLC as Λ_{Defect} was varied from Λ_{defect} = 1000 to 400 nm. In this case, a photonic band is not observed but the PBG itself is seen to exhibit a shift, the shifting amount

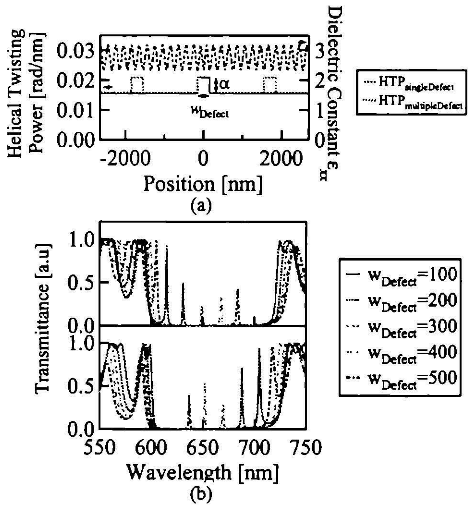

FIG 2. (a)The distribution of the HTP and the dielectric tensor when single or multiple defect layers are introduced. (b) The transmission spectra of the ChLC with a single defect layer ($\alpha = \pm0.3$) for various w_{Defect}.

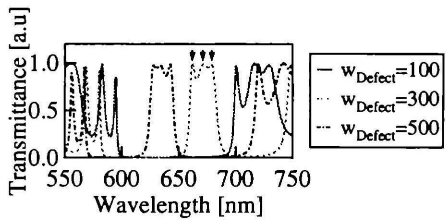

FIG 3. The transmission spectra of the ChLC with multiple defect layers ($\alpha = 0.3$) introduced at Λ_{Defect} = 1700 nm. A blue shift is observed as the layer width is increased.

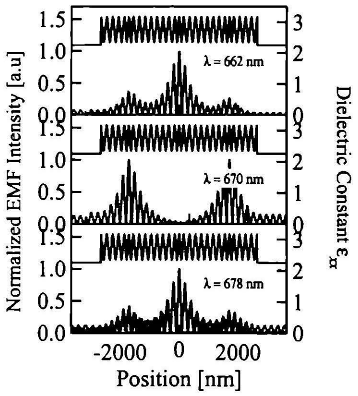

FIG 4. The transmission spectra of the ChLC with frequent thin defect layers (α=0.3). Shift of the PBG is observed by introduction of defects.

depending on how frequent the modulation appears. This result is very characteristic of the ChLC that introducing defects where light would normally localize, results in the shifting of the PBG itself. A tunable PBG is realized by introduction of multiple thin (less than $p_0/2$) HTP defect layers.

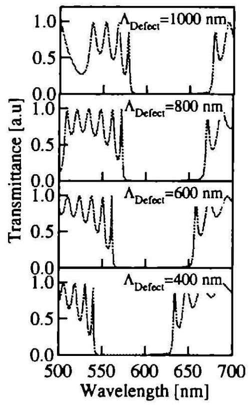

FIG 5. The transmission spectra of the ChLC with frequent thin defect layers (α=0.3). Shift of the PBG is observed by introduction of defects.

CONCLUSIONS

We have introduced various structural modulations in a typical ChLC structure and investigated its effect on its transmission properties. A single defect mode is observed when a single defect layer is introduced in the ChLC, and its wavelength is tunable by adjusting the defect layer length. For the case when p_0 = 400 nm, L = 5300 nm and α = 0.3, the defect mode can be shifted from the longer end of the PBG to the shorter end by introducing a defect layer of approximate width 800 nm.

When multiple defects were introduced, the defect mode split into a band with the number of peaks corresponding to the number of defects introduced in the system. Tuning of the transmittance band was observed also by varying the defect layer length, and for wavelengths in the transmission band the coupling of the EMF between each defect site was observed. On the other hand, when numerous thin defect layers were introduced into the ChLC, shifting of the PBG itself was observed. The amount of PBG shift was dependent on how frequent the modulation was introduced, and the shift seemed continuous.

As we have seen, a phase defect introduced in the chiral periodicity of the structure was seen to affect the transmission property of the ChLC in two distinct ways, depending on how the structure is modulated. Further investigations of defect engineering may lead to realization of self-organizing smart materials.

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