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Omnidirectional Reflection Band of One-dimensional Periodic Structure (1DPS) of Si/SiO_2 with Defect Mode of Nematic Liquid Crystal (5CB)

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ABSTRACT: *In this paper, an omnidirectional reflection band of a one-dimensional periodic structure (1DPS) of Si and SiO_2 with a nematic liquid crystal (5CB) as a defect layer, i.e., $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$, is investigated. The geometry of the 5CB molecules NLC is optimised with the help of density functional theory (DFT) using Gaussian 09 Software packageA02 and the order parameter (S) of the 5CB molecules is calculated. The S value for the 5CB molecules is found to be 0.53 for the range of the applied electric field and confirms the nematic phase of the liquid crystal at the microwave region. By taking average of the ordinary and extraordinary refractive indices of the 5CB molecules NLC, the refractive index has been calculated. The optical properties of the 1DPS of Si and SiO_2 with a 5CB molecules NLC defect layer are calculated to study the optical defect mode as well as the bi-channelled omnidirectional reflection behaviour of the 1DPS $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ and tuned by the electro-optic property of 5CB NLC. Such omnidirectional reflecting behaviour of the considered structure may be used to design b-channelled omnidirectional reflector and defect mode filter and others.*

Keywords: Nematic liquid crystal, 5CB, 1DPS, omnidirectional reflection band, DFT

1. INTRODUCTION

Photonic crystals (PCs) are a unique class of optical media which have a periodic arrangement of dielectric materials in one-dimension (1D), two-dimension (2D) and three dimensions (3D). Photonic crystal has the special property of the optical band gap and such property can be used in optical devices. Generally, the transmission property of the photonic crystal depends on the geometry and the refractive index of dielectric materials. PCs exhibit the photonic band gap (PBG) region in transmission spectra of the photonic crystal. The PBG is a forbidden region where no frequency or electromagnetic wave can propagate inside the crystals. Due to such characteristics in the transmission spectra, PCs are very useful in optoelectronic devices.[1,2] It has been shown that 1D photonic crystal can be used as a reflector for transverse electric (TE) and transverse magnetic (TM) modes with the variation of incident angle. The common reflection bands found in reflection spectra for both TE and TM polarisations are called an omnidirectional reflection bands and can be used to fabricate omnidirectional reflectors and filters.[3–6]

Liquid crystals (LCs) are organic molecules having an intermediate phase between liquid and crystalline state. LCs have liquid like flow property and crystals like periodic arrangement of atoms or molecules. LCs have the nonlinear optical characteristics and various applications in display technology, nonlinear devices, optical devices, optoelectronic devices, etc. Generally, LCs are found in three types: lyotropic, thermotropic and metallotropic. But we are interested to study the electro-optical properties of the thermotropic liquid crystal which are responsible on the application of temperature and electric field, and such LCs changed their phases and optical properties when we apply the temperature and the electric field. Therefore, thermotropic liquid crystals exhibit different phases are called nematic, cholesteric and smectic phases.[7–10] Liquid crystal has a large dielectric anisotropy and response to the temperature and electric field. On the basis of dielectric anisotropy of the liquid crystal, the photonic crystals have been proposed by considering opal or inverse opal infiltrated with liquid crystals.[11–15] PCs with a defect layer of liquid crystal shows tunable transmission with defect mode wavelength in PBG region and such defect mode wavelength peaks can be controlled by application of electric field. The application of low voltage is demonstrated by the electro-optic switching, the defect mode lasing in 1D periodic structure with liquid crystals as a defect layer.[16–20] The liquid crystal are anisotropic molecules having extraordinary refractive (n_e) and the ordinary refractive indices (n_o). Another hand, order parameter (S) is a very important parameter for the liquid crystal to characterise the phase of liquid crystals. The value of S is 0 and 1 for pure liquid state and perfect crystal state, but S lies between 0 and 1 which indicates the liquid crystalline state, respectively. For nematic phase of the liquid crystal, order parameter is found to be near about 0.5. The S value of LC depends upon the director tilt angle and the polarizability of liquid crystal molecules.[21–23]

In the present paper, we studied the omnidirectional reflection properties of a periodic structure with liquid crystal (5CB) as a defect layer where liquid crystal sandwiched between the semi-finite periodic structures of the Si and SiO_2 materials, i.e., $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$. The geometry of the 5CB molecule was optimised by density functional theory (DFT) using Gaussian 09 software package A02 and the order parameter of the 5CB molecule was calculated to characterise the phase of the LC. The optical properties of the 1DPS $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ were studied using transfer matrix method (TMM) and such optical properties is useful to design omnidirectional reflector with defect mode filter as well as tunable bandwidth application.

2. THEORY AND METHODOLOGY

Firstly, we optimised the geometry of 5CB molecules using Gaussian 09 Software package A02 with the help of DFT using B3LYP method and 6-31G** basis set.[24–27] Further, we calculated S value of the 5CB molecules, which is an important parameter to explain the phase behaviour of liquid crystals. The calculated S value of the 5CB liquid crystal is found to be 0.53 which shows the nematic phase of 5CB liquid crystal in the microwave region. Now, 5CB NLC is inserted between the semi-finite periodic structure of the Si and SiO_2 materials in one direction as shown in Figure 1.

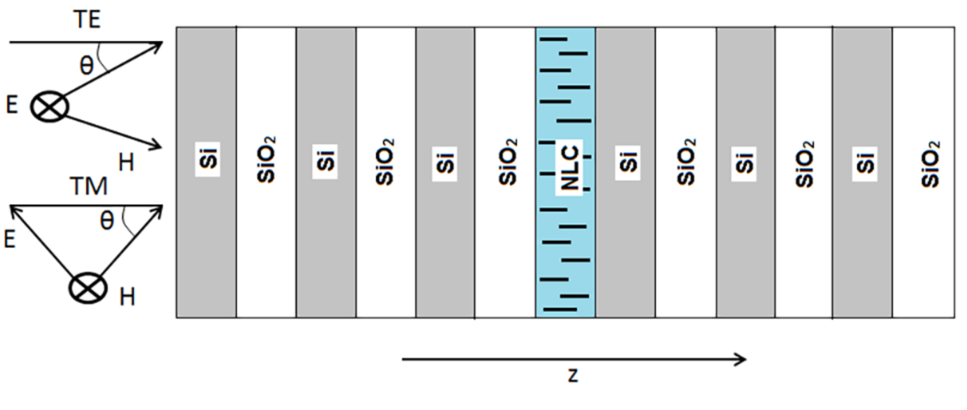

Figure 1: Schematic diagram of 1D periodic structure containing the defect of nematic liquid crystal with structure $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$.

To calculate the optical properties of the periodic structure of Si and SiO_2 with 5CB NLC as defect layer, we have considered the refractive indices of the Si and SiO_2 materials to be 3.4 and 1.5, respectively. However, the refractive index of liquid crystal depends on the extraordinary and ordinary refractive indices of the liquid crystals. In our calculations, we have considered the average refractive index of the liquid crystal (n_{LC}) represented as Equation 1. The thicknesses of dielectric layers Si and SiO_2 follow the relation represented as Equation 2, where wavelength (λ) is taken as 0.55 μm for propagation of the wave inside the periodic structure. The thickness of the liquid crystal layer is taken as 100 nm. The extraordinary (n_e), ordinary (n_o) and the average refractive indices of liquid crystal are 1.81, 1.56 and 1.64, respectively.[28] Therefore, the refractive index of the LC is:

$$n_{LC} = \frac{2n_o + n_e}{3} \tag{1}$$

For the maximum transmissions, the periodic structure follows the condition which is represented as follows:

$$n_{Si} d_{Si} = n_{SiO_2} d_{SiO_2} = \lambda/4 \tag{2}$$

To study the optical properties of the structure $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$, we have used the TMM.[29] The TMM for a single dielectric layer is given by Equation 3. The total transmission and reflection of the proposed 1D periodic structure are given by Equations 4 and 5. The transfer matrix, M, for the Nth layer is given by:

$$M = D_0^{-1}\left[\prod_{i=1}^{N} D_i P_i D_i^{-1}\right] D_s \tag{3}$$

where $D_i = \begin{bmatrix} 1 & 1 \\ n_i \cos\theta_i & -n_i \cos\theta_i \end{bmatrix}$, $P_i = \begin{bmatrix} \exp(i\phi_i) & 0 \\ 0 & \exp(-i\phi_i) \end{bmatrix}$

The transmittance and reflectance of the considered periodic structure with 5CB NLC as defect layer are given as:

$$T = \frac{(n_s \cos\theta_s)}{(n_0 \cos\theta_0)} \left| \frac{1}{M_{11}} \right|^2 \tag{4}$$

$$R = \frac{(n_s \cos\theta_s)}{(n_0 \cos\theta_0)} \left| \frac{M_{21}}{M_{11}} \right|^2 \tag{5}$$

where $\phi_i = 2\pi n_i d_i \cos\theta_i/\lambda$; D_i is the dynamical matrix; P_i is the propagation matrix for the ith layer of periodic structure; n_i and d_i are the refractive index and layer thickness of ith layer, respectively, θ_i is the incident angle for ith layer; λ is the wavelength; N is the number of layers; and subscript s stands for subtracting layer in consider structure. D_0 and D_s stand for the dynamical matrix for air and subtract layers, respectively.

3. RESULTS AND DISCUSSION

It is found theoretically that the maximum value of the order parameter of 5CB molecules is 0.53 for the range of electric field, i.e., 0.05–0.12 a.u. The 5CB molecules show the nematic phase of the LC. Therefore, 5CB molecules are treated as the nematic liquid crystal 5CB NLC. The behaviour of order parameter (S) of the 5CB NLC under electric field is shown in Figure 2.

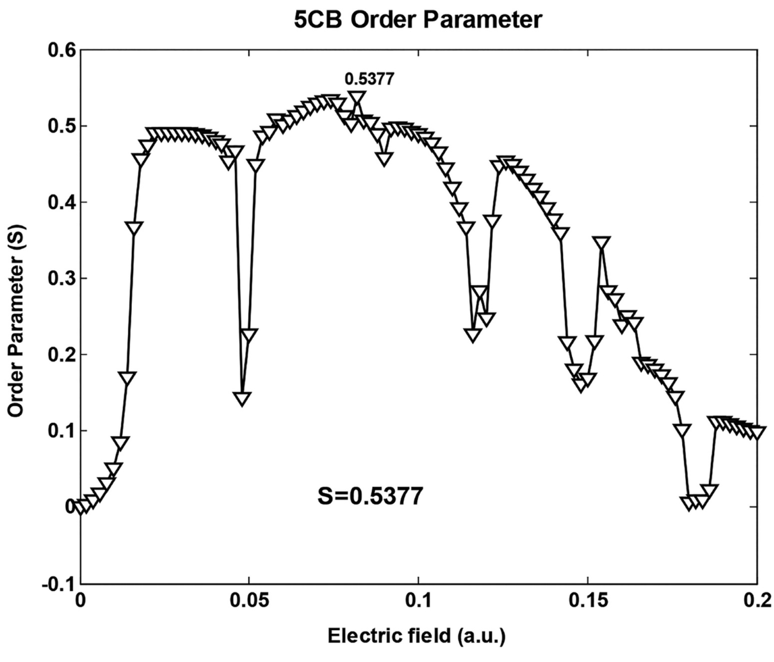

Figure 2: Order parameter of the 5CB molecules (NLC) under applied electric field (a.u.).

The average refractive index and the thickness of the 5CB NLC are taken as 1.64 and $d_{NLC} = 100$ nm, respectively. The effect of electric field on the 5CB NLC is analysed by considering the periodic layers of Si and SiO_2 materials with 5CB NLC as defect layer, i.e., $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ structure as shown in Figure 1.

The transmission and reflectance of the considered structure are calculated using the TMM method.[29] The refractive indices and thicknesses of Si and SiO_2 are $n_{Si} = 3.4$, $n_{SiO2} = 1.5$, $d_{Si} = 40.4$nm, and $d_{SiO2} = 91.66$ nm, respectively. These data are used to calculate the transmittance behaviour of a 1D periodic structure of Si/SiO_2 materials without and with a defect layer of 5CB NLC, i.e., $(Si|SiO_2)^6$ and $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$.

The transmission of the periodic layers of Si/SiO_2 materials without and with a defect layer of the 5CB NLC versus incident angle for TE mode are shown in Figure 3. From Figure 3(a), it can be seen that there exists a photonic band gap (PBG) region between 0.4 µm and 0.75 µm wavelength for periodic structure $(Si|SiO_2)^6$. This PBG region varies with incident angles (θ) of the electromagnetic wave. The transmittance of the periodic structure with 5CB NLC as defect, i.e., $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$, as shown in Figure 3(b). There is an enhancement in the PBG region with defect mode wavelength peak at 0.5 µm in the transmission spectra. The behaviour of defect mode wavelength peak with the incident angle is also investigated. It can be easily seen from Figure 3(b) that a shifting of defect mode peak is obtained towards lower wavelength with low transmission as the incident angle increases. The shifting of the defect peaks is shown at three different incident angles i.e. 0°, 45° and 89°. This study shows that the defect mode of the 5CB NLC in the periodic structure alters the PBG region due to the presence of the defect layer in the symmetric periodic structure $(Si|SiO_2)^6$.

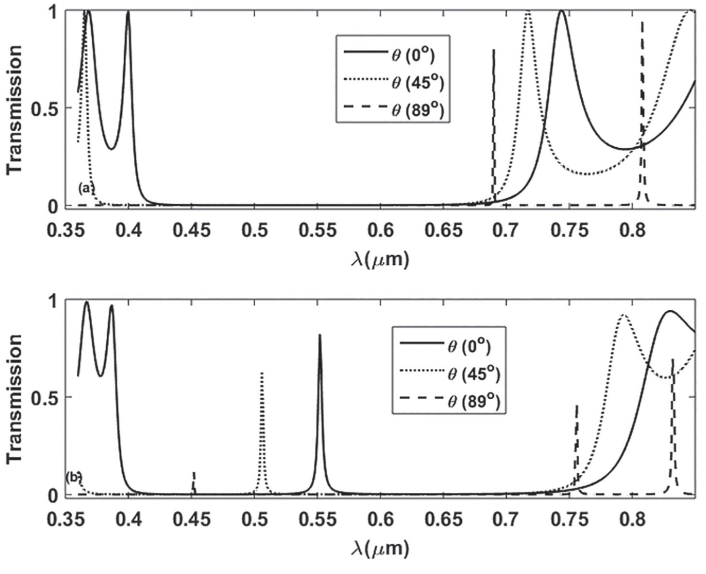

Figure 3: Transmission versus wavelength at different incident angles for (a) $(Si|SiO_2)^6$, and (b) $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$.

Figure 4 shows the transmission spectra of the periodic structure with 5CB NLC as defect, $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$, for both TE and TM modes at three different incidence angles, i.e. 0°, 45° and 89°. For TE mode, the defect mode wavelength peak with lower transmission at high incidence angle shifts towards low wavelength as shown in Figure 4(a). Similar behaviour find for TM mode which is shown in Figure 4(b). Although, the defect mode wavelength peak for the TM mode is shifted towards the low wavelength region for high incidence angle. But the high transmittance is obtained for TM mode in comparison to TE mode.

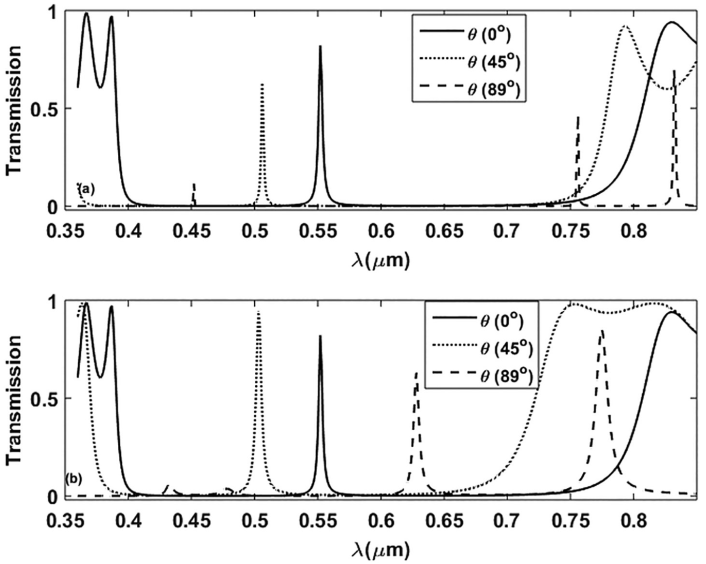

Figure 4: Transmission versus wavelength of $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ at different incident angles, i.e., 0°, 45° and 89° for (a) TE mode, and (b) TM mode.

Now, the omnidirectional band gap (OBG) of the periodic structure is calculated by taking common PBGs for TE and TM modes. Figure 5 clearly shows the PBG for TE mode which is larger than TM mode. The common PBG for both TE and TM modes can be used as an omnidirectional reflector at microwave region. Similarly, we have studied the PBG for the $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ structure for both modes. Such periodic structure has also OBG with a defect mode wavelength peak in PBG as shown in Figure 6. The defect mode can be used as a bi-channel omnidirectional reflector at microwave wavelength region.

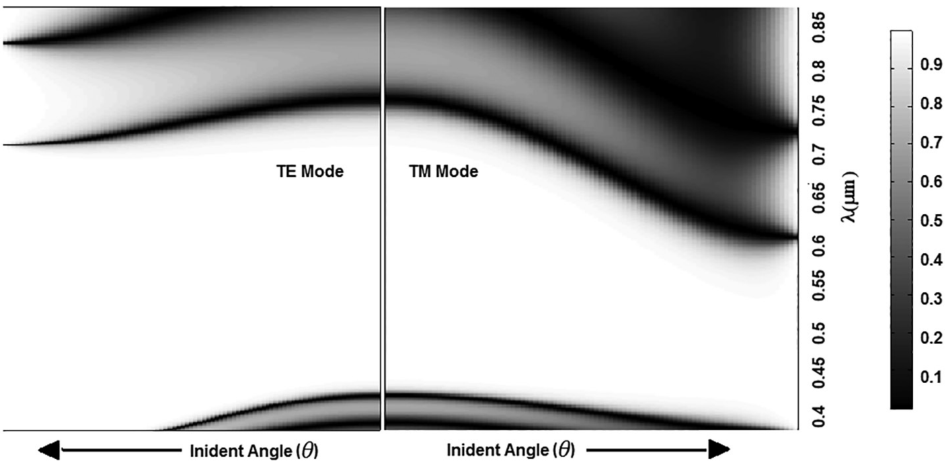

Figure 5: 2D image of wavelength versus incident angle of the $(Si|SiO_2)^6$ for TE and TM mode (full-coloured illustration is available in the digital version).

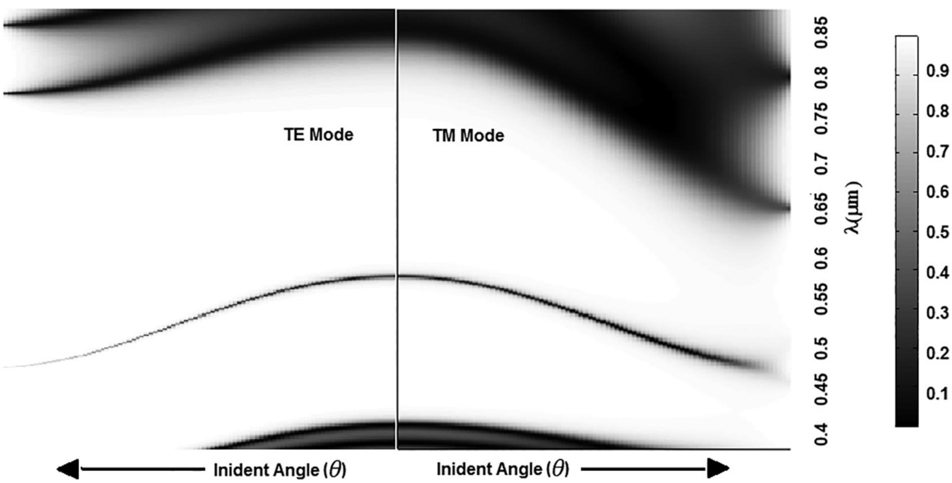

Figure 6: 2D image of wavelength versus incident angle of the $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ for TE and TM mode (full-coloured illustration is available in the digital version).

The PBG and bi-channel property of the $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ are easily understand with 3D image of the reflectance versus wavelength at different incident angles. Figure 7 shows a bi-channel omnidirectional reflection band of the periodic structure $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ and concludes that the reflectance of defect mode wavelength peak for TE mode decreases for the high incident angle. But the reflectance of defect mode wavelength peak for TM mode increased with higher incident angle where the reflectance again decreased at 60° incident angle. Comparative 3D image of reflectance spectra for $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ is shown in Figures 7 and 8 for TM and TE modes which shows that PBG regions are different, respectively.

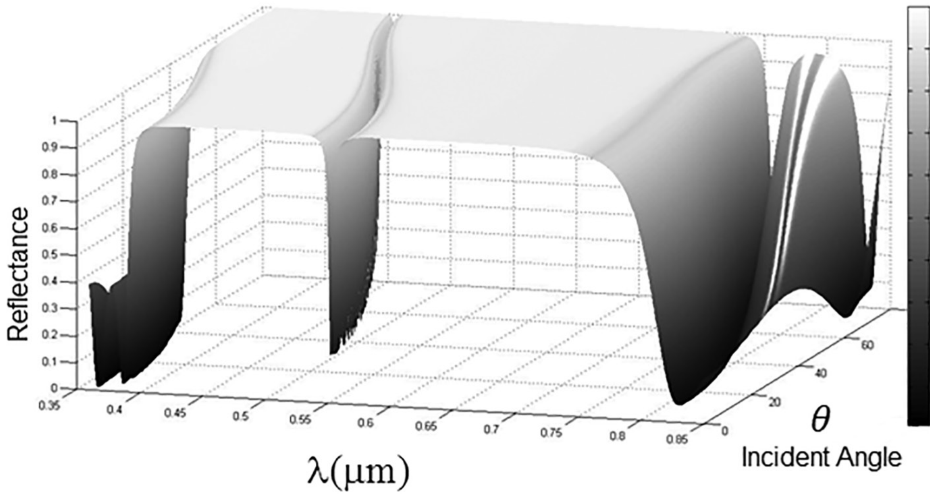

Figure 7: 3D image of reflectance versus wavelength $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ with different incident angles for TE mode (full-coloured illustration is available in the digital version).

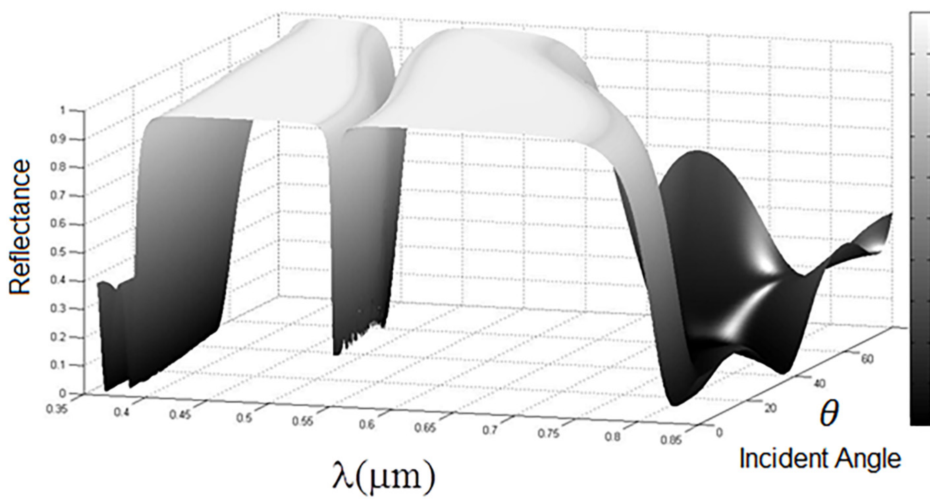

Figure 8: 3D image of reflectance versus wavelength of $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ at different incident angles for TM mode (full-coloured illustration is available in the digital version).

Further, transmissions of defect mode wavelength peak of the periodic structure $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ are studied with high incident angle. The transmission for TE mode is continuously decreased with high incident angles but the transmittance in cases of TM mode is increased initially with high incident angle and reached to the maximum value to 60° incident angle and then transmission further is decreased as shown in Figure 9.

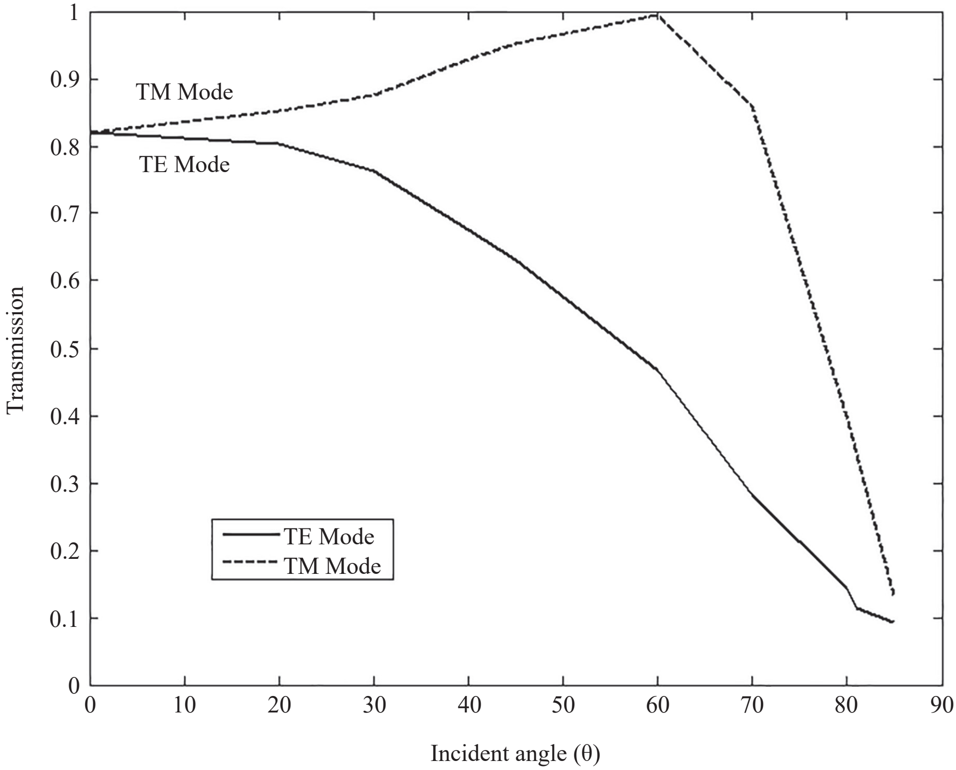

Figure 9: Comparative transmission of defect peak versus incident angle for TE mode and TM mode for $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ structure.

4. CONCLUSION

It is well known that the photonic crystals are very useful to design the optical devices due to exhibiting of the PBG in the transmission spectra. The PBG materials are used to fabricate optical devices like filters, omnidirectional reflectors, etc. In our paper, we have chosen 5CB NLC as a defect layer in the periodic structure of Si and SiO_2 and have calculated the order parameter of the 5CB NLC with help of Gaussian 09 Software package A02. The calculated order parameter shows that the 5CB NLC is the nematic phase for 0.05–0.12 a.u. electric field. By taking the average of the ordinary and the extraordinary refractive indices of 5CB NLC, average refractive index of the 5CB NLC is calculated. The optical properties of the 1DPS of Si/SiO_2 with defect mode of the 5CB NLC are calculated using the well-known TMM. A 100% reflectance of the one-dimensional periodic structure of Si/SiO_2 dielectric materials for TE and TM modes shows the omnidirectional reflection behaviour at the microwave region. Periodic structure $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ has bi-channelled omnidirectional reflection band when defect 5CB NLC is introduced as defect layer in the symmetric semi-finite periodic structure of Si and SiO_2. The omnidirectional reflecting behaviour with defect mode of the 1DPS $(Si|SiO_2)^3|NLC|(Si|SiO_2)^3$ may be considered to design bi-channelled omnidirectional reflector which is tuned by the electro-optic behaviour of the 5CB NLC. The 100% reflectance of the considered structures may be used to fabricate the photonic for omnidirectional reflector and filter.

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