3D modelling of carbon nanotubes and liquid crystal based nano-photonic device

Kanghee Won, Ranjith Rajasekharan, Haider Butt, Qing Dai, Timothy D. Wilkinson*

Department of Engineering, Centre of Molecular Materials for Photonics and Electronics,

University of Cambridge, 9 J.J. Thomson Avenue, Cambridge, CB3 0FA,

United Kingdom

ABSTRACT

In this study, we present electric field (E-field) modelling and experiment of arrays of vertically grown carbon nanotubes as three dimensional electrode structures, in order to address liquid crystal molecules in a switchable nano-photonic device. The electric field spawned by the nanotube electrodes is used to align the liquid crystal molecules to generate a gradient refractive index profile across the device. It was observed that multiple nanotube groups generated wide and symmetrical electric fields compared to other geometries. We have utilized nano-photonic devices based on the simulation results and compared them with experimentally obtained electro-optic characteristics. These devices have many applications in voltage reconfigurable micro-optical systems.

Keyword: nanophotonic; carbon nanotube; nematic liquid crystal; electro-optic devices

1. INTRODUCTION

Nematic liquid crystals are anisotropic materials with calamitic molecules, which generally align in a preferred direction. At the same time, there is a strong interest in novel and improved nematic devices. Therefore, numerous efforts have been attempted to change the electro-optic characteristics and the carbon nanotubes (CNTs) have been studied due to their strong interaction with liquid crystals and outstanding electrical properties [1-3]. An electrically switchable micro-optical device based on a sparse array of multi-walled carbon nanotubes (MWCNTs) was developed [4] and different numbers of nanotubes in groups were recently grown on a transparent quartz substrate.

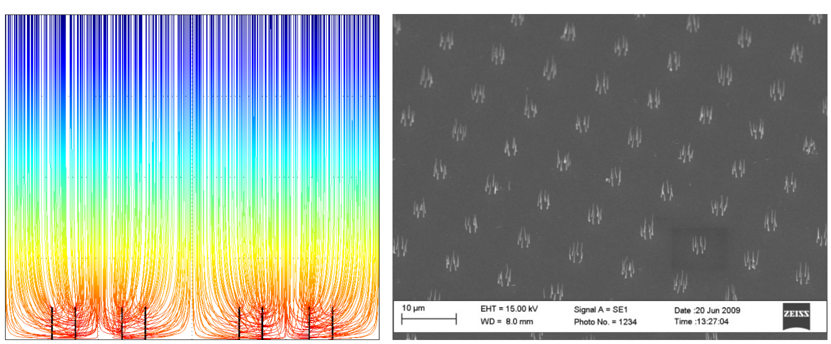


Figure 1. a) Simulated electrical field profile surrounding the carbon nanotube in groups of six (2 μm high) with an applied field of 10 V μm^{-1} [4], and b) Image of sparse array of nanotubes on quartz substrate with nanotube group spacing of 10 μm [5].

As shown in Fig. 1, a very unusual electric field profile is produced when a voltage is applied to the nanotube electrodes. It is observed that the liquid crystal molecules follow the direction of the field for the case of a positive dielectric anisotropy. Determination of the liquid crystal behaviour is crucial for future development of these devices. However there is yet to be a methodical investigation that analyzes the exact behaviour of LC molecules considering the three-dimensional structure. Also, a narrowly defined nonlinear region is found around a single nanotube, whereas groups of nanotubes give more expanded and wider regions.

In this article, the behaviour of the liquid crystal director is investigated using a liquid crystal modelling simulation programme. The results are compared to the experimental data and the effect of nanotubes within a hybrid LC-CNT cell is reviewed in terms of the optical characterisation.

2. DEVICE STRUCTURE AND OPERATING MECHANISM

The device consists of two substrates with an interspacing of 20 µm. The top substrate, 0.5 mm thick borosilicate glass, was coated with transparent and electrically conductive indium tin oxide (ITO) on its inner surfaces. The multi walled carbon nanotubes (MWNTs) of 50 nm in diameter and 2 µm in height were mounted on the lower substrate to act as individual electrodes. A positive dielectric anisotropy nematic LC mixture, BLO48 from Merck, is sandwiched between the two layers as shown in Fig. 2. The material parameters of BLO48 liquid crystal mixture which were used for the director profile simulation are listed as follows: birefringence, $\Delta n = 0.2627$ at $\lambda = 523$ nm; dielectric anisotropy, $\Delta\varepsilon = 16.8$; elastic constants, $K_{11} = 15.5$ pN, $K_{22} = 12$ pN, $K_{33} = 28$ pN, and rotational viscosity $\gamma_1 = 0.047$ Pa-sec.

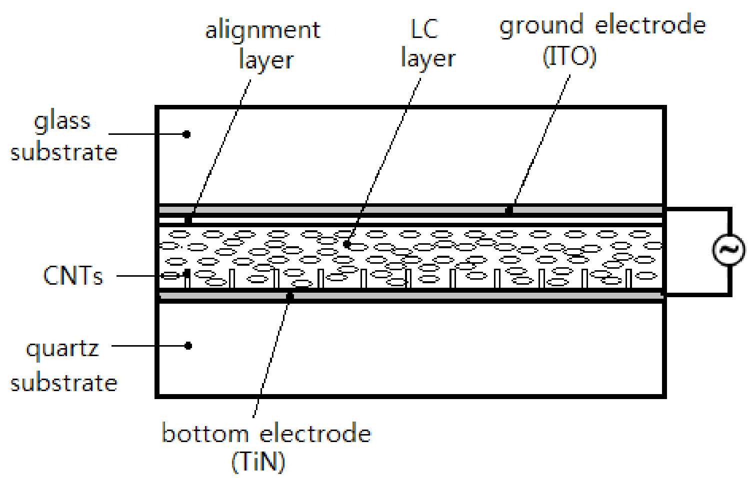


Figure 2. Schematic of a LC-CNT device

We used a polyimide (AM4276 from Merck) as a homogeneous LC alignment layer on the top substrate which yields a low pre-tilt angle of 2 ° after general rubbing but no alignment was applied to the bottom substrate due to the nanotube array. The electrode materials used for the top substrate and the bottom substrate were ITO and titanium nitride (TiN), respectively. When a voltage is applied to the bottom electrodes, a symmetric inhomogeneous electric field appears in the vicinity of the nanotubes as shown in Fig. 1 a.

3. EXPERIMENTAL AND SIMULATED RESULTS

Having some knowledge of the LC director profile in our device is essential for its proper utilisation and optimisation. We employed a commercial LCD simulator known as *TechWiz LCD 3D* to calculate the LC director orientations and the electro-optic properties of the LC-CNT device.

The layers and structures employed in the simulation tool were based on the actual device structure. The liquid crystal director profile was calculated based on the Ericksen-Leslie equations. The boundary condition of the top electrode, ITO, was set to ground (0 V) whereas the bottom substrate electrodes, TiN and CNT, were set to sweep mode voltage, which changed the voltage simultaneously from 0 V to 10 V and performed the calculations at each voltage. As mentioned earlier, only the top substrate was coated with low pretilt polyimide and no alignment layer was applied to the bottom substrate in the actual device. However, it was reported that the LC alignment can be predicted based on continuum theory [6, 7]. If the LC molecules are anchored parallel to the substrate, then it will always result in a parallel orientation throughout the LC layer. For this reason, it is assumed that the LC molecules keep their position according to continuum theory, the same angles of a tilt and a azimuthal ($\theta = 2$ °, $\varphi = 0$ °) near to the top surface were used to define the initial distribution of director on the bottom surface in the simulation. The LC director was horizontally aligned in the absence of an electric field and the defects are shown around the CNTs as shown in Fig. 3 b.

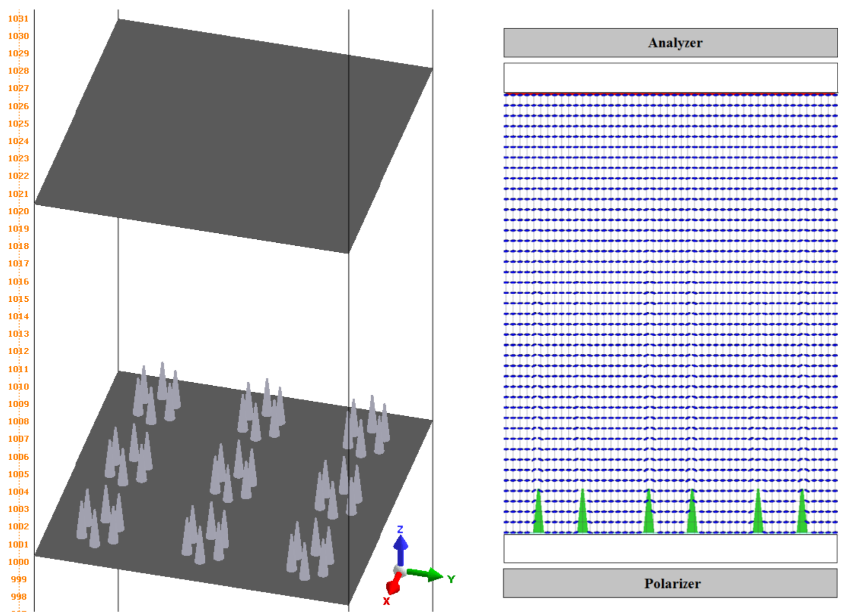


Figure 3. a) Schematic diagram of a hybrid LC-CNT device, and

b) Two dimensional cross-sectional view of a planar aligned LC-CNT device structure with no applied voltage.

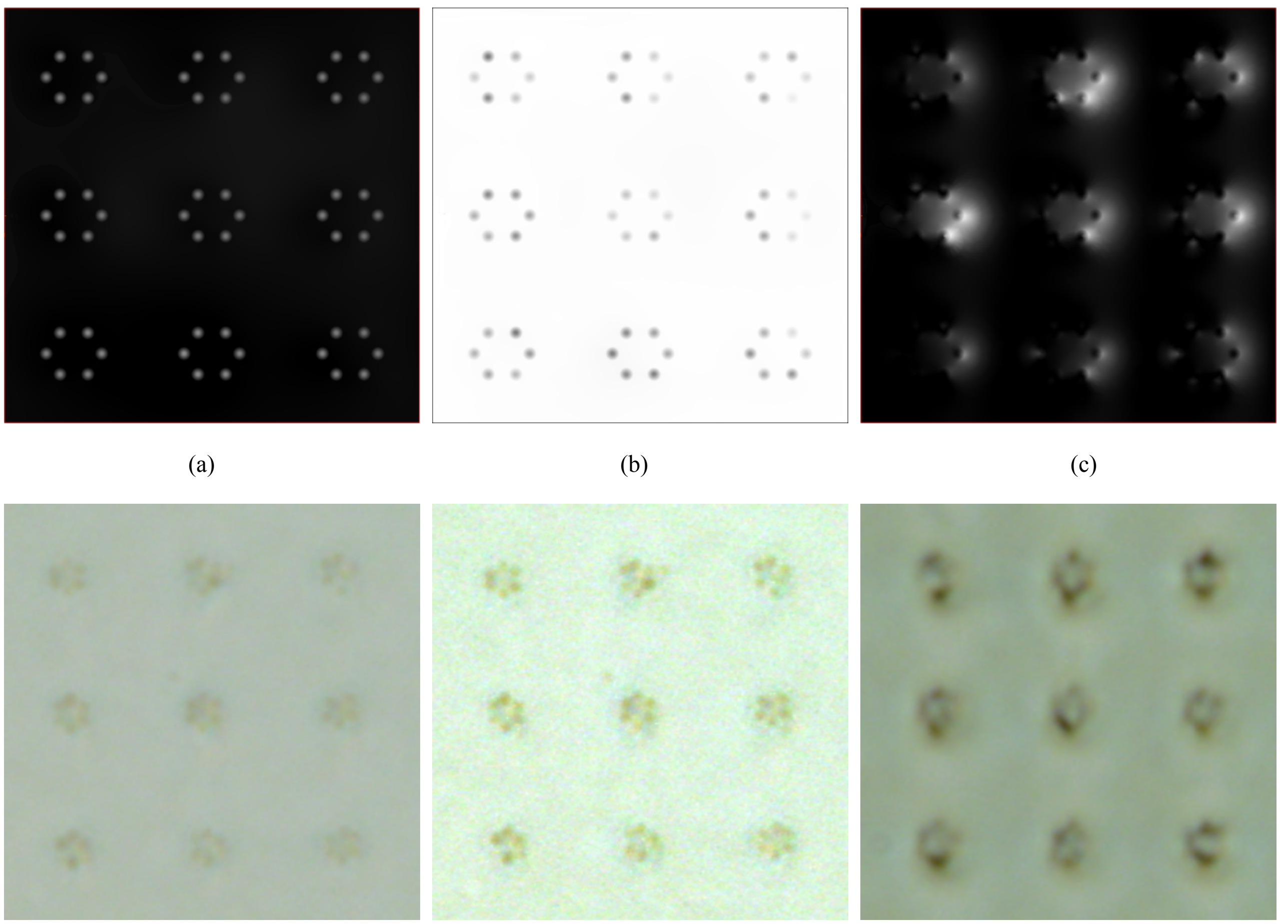
The optical characteristics of the LC-CNT device were simulated to analyse the transmittance. The transmittance of the LC cell through crossed polarizers can be defined as follows [8].

$$T = 1/2 \sin^2 (2\text{Ø}\Delta) \sin^2 (\pi \Delta nd / \lambda)$$

where ΔØ is the twist angle relative to the transmission axis of the polarizer due to the applied field, λ is the wavelength of the incident light, and Δnd is the retardation of the LC cell.

For the crossed polarizers, the analyzer is oriented 90 ° with respect to the polarizer, and the orientation of the LC-CNT cell is rotated 45 ° with respect to the polarizer and analyzer. Two different kinds of LC cells were simulated, with all undoped and 6 nanotube array cells operating in the normally white (NW) mode. The 633nm wavelength of an input light source was applied for transmission measurements which is the same wavelength as a polarized He-Ne laser that is used in our experimental work [5]. The performance of the hybrid LC-CNT device is simulated using a 4 x 4 extended Jones matrix. The transmittance characteristic as function of voltage was accomplished and it was compared to the experimental data.

The arrays of nanotubes appeared as dots due to defects near at the nanotubes. When the applied voltage was increased from 0 V to 6 V, many of the black and white mixed states were observed. The first minima and the first maxima optical textures are shown in Fig. 4 (a) and (b), respectively. Above the critical voltage, light leakage caused from the deformation of the LC director was observed as shown in Fig. 4 (c). This is because nanotubes can disperse the LC alignment due to their translational motions. Also, experimental optical textures are captured at different voltages as shown in Fig. 4 (d)-(f).



(a) (b) (c)

(d) (e) (f)

Figure 4. Simulated (a-c) and experimental (d-f) optical textures for a hybrid LC-CNT cell at various voltages

(a - 2.2 V, b - 3.1 V, c - 10 V, d - 1 V, e - 0.5 V, f - 4.5 V)

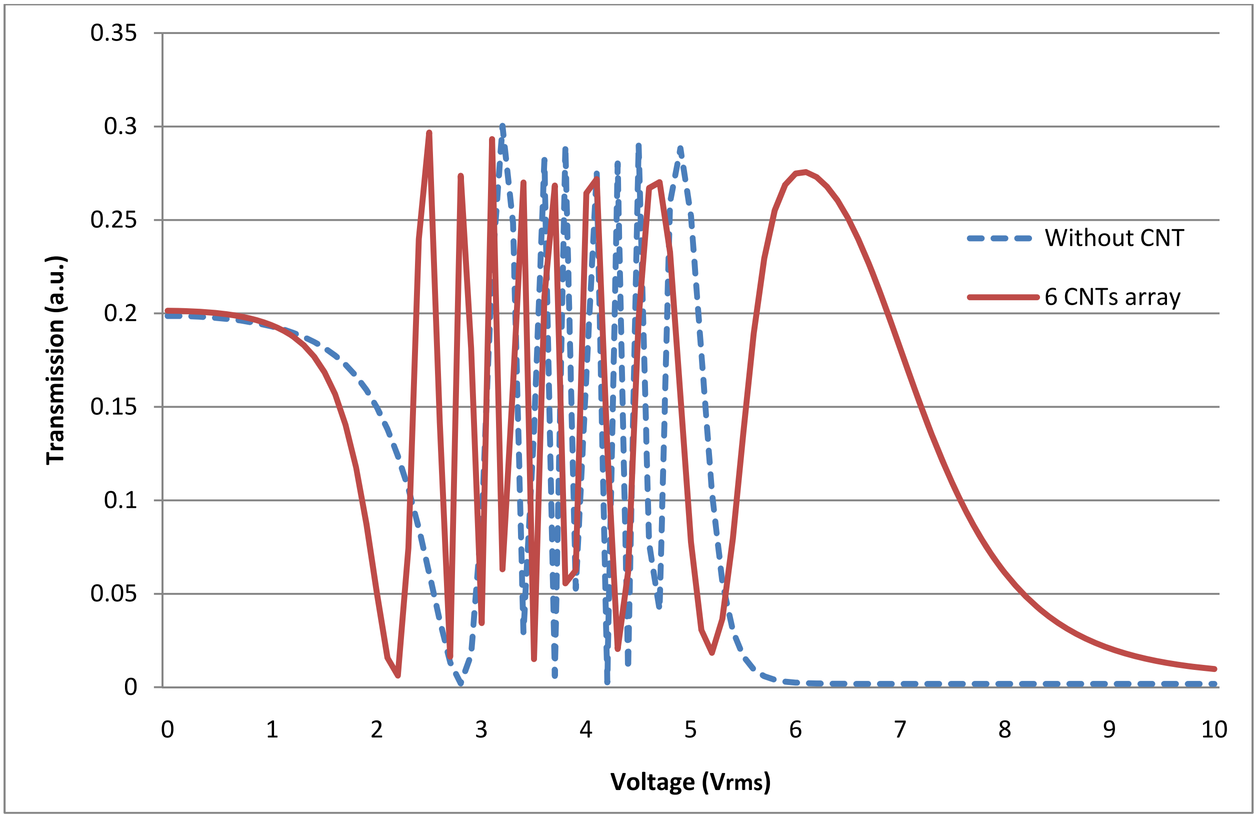
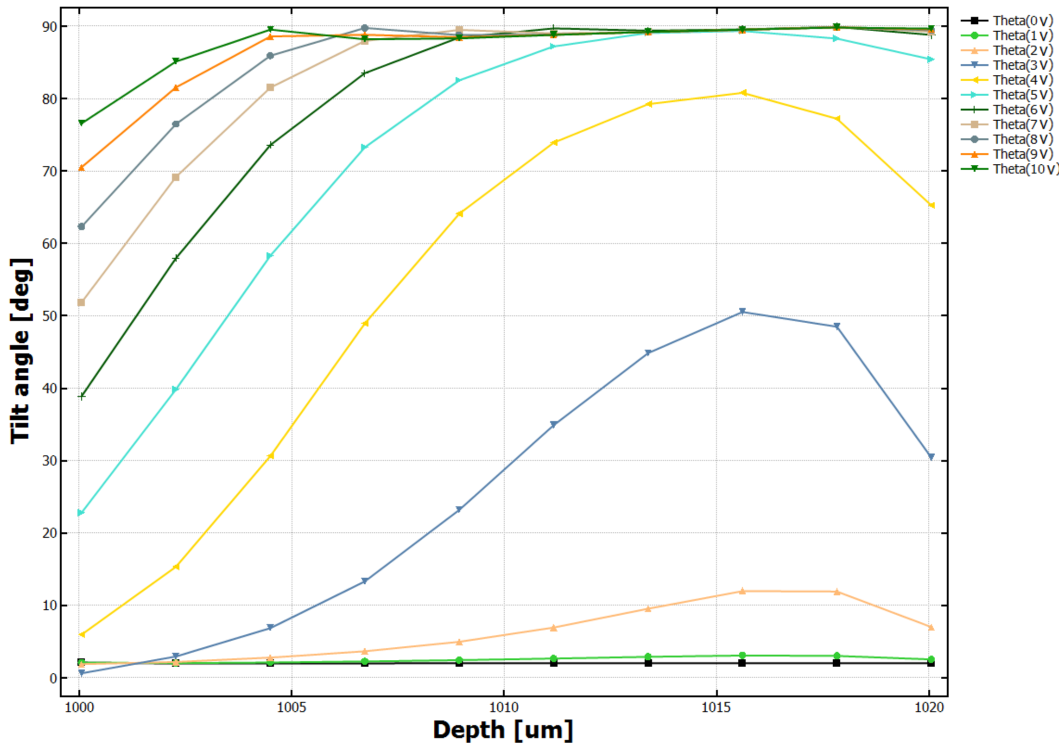


Figure 5. Simulated T-V characteristic of the transparent nano-photonic device

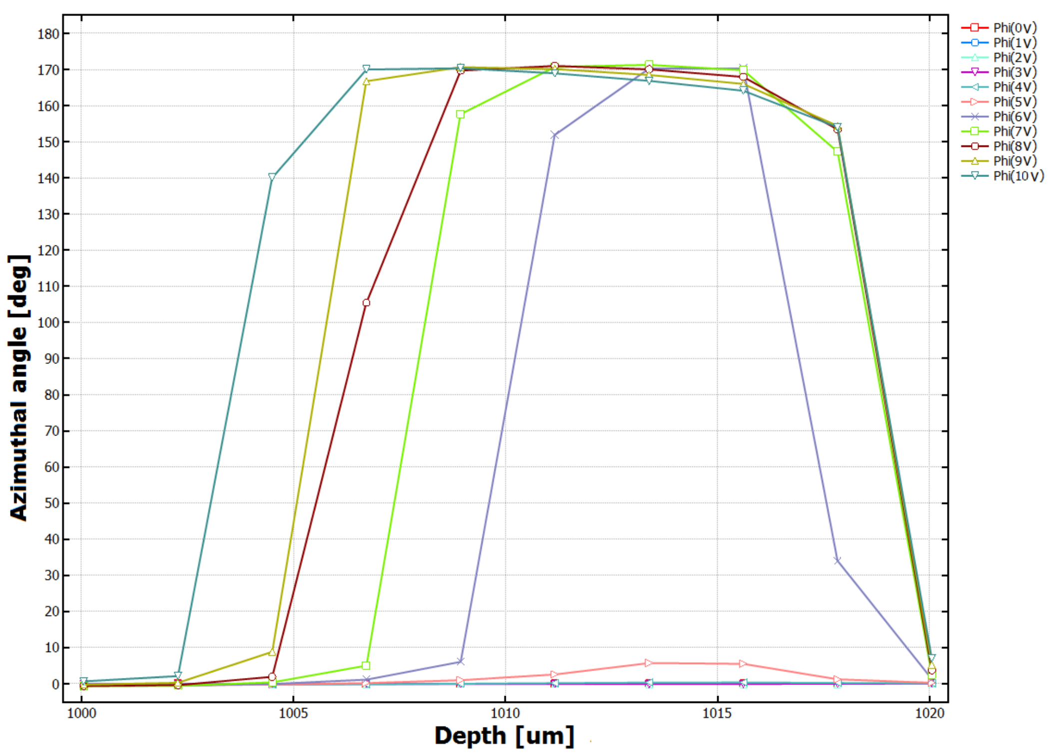
Fig. 5 shows the transmittance versus applied voltage (T-V) curve of the liquid crystal cells for two different cases; one is a liquid crystal cell with 6 nanotube array and the other is without nanotubes. As the applied voltage increases the reorientation process undergoes several maxima and minima of transmitted intensity with different configurations of phase retardation profiles. These simulation results are verified experimentally and it was also found that our LC-CNT device with 6 nanotube array has also several maxima and minima in the T-V curve [5]. For NW mode, the threshold voltage V_{th} and the driving voltage V_{on} were defined as the voltages where the transmission decreased to 90% and to 10% of the initial value at no applied voltage, respectively. It was observed that V_{th} (V_{on}) = 1.56 (2.66) and 1.31 (2.07) V for the undoped and the 6 nanotube array doped cell, respectively. It is clear that the liquid crystal cell with the nanotube array reduces the threshold voltage compared to the pure liquid crystal cell due to the greater electric field as a result of the high aspect ratio nanotubes (diameter of 50 nm and length of 2 μm) [9]. In terms of the driving voltage, the first minima in the transmission were found at 2.8 V and 2.2 V for the undoped and the CNT-doped cell, respectively. This is because the Gaussian shaped electric field caused from the CNT resulted in a horizontal alignment of the liquid crystal molecules at a lower voltage. For V > 10, virtually all the molecules were reoriented by the electric field so that the liquid crystal director was perpendicular to the substrates within a 6 nanotube array, whereas the same phenomenon was found to occur for V > 6 within the undoped cell. This is because the greater electric field is required to reorient the liquid crystal molecules which are anchored close to nanotubes, in order to achieve homeotropic alignment. Moreover, there are still some defects around the nanotubes as evident in Fig. 3 b. Hence, it is not easy to totally vertically dispersed in the liquid crystal molecules with the nanotube array and the maximum transmission of the LC-CNT cell is slightly reduced compared to the undoped cell.

The liquid crystal director deformations of 6 nanotube array LC-CNT cell under different applied voltages are shown as functions of the depth of a liquid crystal cell in Fig. 6.



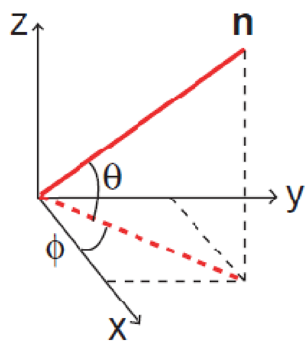
Tilt angle [deg]
Depth [um]
Theta(0V)
Theta(1V)
Theta(2V)
Theta(3V)
Theta(4V)
Theta(5V)
Theta(6V)
Theta(7V)
Theta(8V)
Theta(9V)
Theta(10V)

(a)



Azimuthal angle [deg]
Depth [um]
Phi(0V)
Phi(1V)
Phi(2V)
Phi(3V)
Phi(4V)
Phi(5V)
Phi(6V)
Phi(7V)
Phi(8V)
Phi(9V)
Phi(10V)

(b)



(c)

Figure 6. a) Tilt and b) azimuthal angle of liquid crystal directors at different applied voltage from 0 to 10 V (6 nanotube array), and c) Definition of the tilt angle θ and the azimuthal angle φ.

The liquid crystal director configuration depends on the interaction between elastic forces, external field, and surface treatment. A nematic liquid crystal, which was confined between substrates was considered at z = 1000 µm and z = 1020 µm (where z = 1000 µm defines the location of the bottom electrode, z = 1020 µm defines the location of the top electrode) as shown in Fig. 3 a. The orientation of the liquid crystal director is defined by the tilt angle θ (the angle between the LC director and the x-y plane) and azimuthal angle φ (the angle between the projection of the LC director on the x-y plane and the x axis). In Fig. 6, tilt and azimuthal LC director profiles are displayed for a 6 nanotube array LC-CNT cell with different applied voltage and they were extracted from a distance of 0.1 µm from the nanotubes. It is clear that below critical voltage (2-3V), the director profile is unperturbed and remains uniform. Above this value, the tilt and azimuthal angles begin to change due to a competition between restoring elastic forces and destabilizing torques produced by the electric field, also known as the Frederick transition [10]. Above the threshold voltage, the LC molecules start aligning to the strong electric field produced by the MWCNTs. The maximum director tilt $\theta_{max} = 90$ ° can be found above 5 V in the mid-region of the cell. The tilt angle decreases closer to the top substrate due to the anchoring force. However, with a further increase in applied voltage the bulk of the LC attains a vertical tilt angle of 90 degree due to the increased electro static forces. There is a main difference between the tilt and the azimuthal angles. The azimuthal angle also remains unchanged for voltages below the threshold voltage. However, at the potentials of 4 - 5V the Frederick transition takes place and the molecules align with the curved electric fields. The simulation shows that the molecules appear to rotate about x axis above the 6 V as shown in Fig. 6 b. This is because, when the tilt angle reaches to maximum of θ = 90 °, the surplus electrostatic energies are balanced by rotating the liquid crystal molecules in azimuthal plane.

4. CONCLUSION

In this study, we have investigated the effect of the nanotubes array on the bottom substrate on the optical characteristics and liquid crystal director profiles in our hybrid LC-CNT device by simulation. A non-uniform voltage distribution caused by different nanotube arrays brings unpredictable optical properties and future study on these liquid crystal behaviours is essential. It was found that most of the liquid crystal molecules distortion is introduced from the middle of the cell immediately after the threshold voltage, causing the several maxima and minima in transmitted intensity within a low applied voltage. It is clear that the nanotube array reduced the threshold voltage. Many advantages from the mixture of a liquid crystal and a carbon nanotube may result in promising alternative solutions to conventional devices due to a significant effect on the electro-optic characteristics. Further study of the optimization of different carbon nanotube geometries will result in the improvement of a hybrid LC-CNT device for switchable and adaptive microlens applications.

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