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# Liquid Crystals

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## Gravitational field-induced orientational transition of aligned nematic liquid crystals

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We demonstrate induced orientational transition of liquid crystal (LC) E7 between two optical fibre tips in a gravitational field as a result of minimising the free energy. The LC orientational transition is from a homeotropic state, with respect to fibre tip, to a tilted state as the spacing between two fibre tips is increased. The orientational distortion introduces birefringence in the optical fibre that changes the polarised direction of the output light. At short spacing, the undistorted homeotropic orientation of LC is preferred. However, at longer spacing, a distorted orientation is preferred. Once the LC director profile is known, a Finite Difference Time Domain method is used to calculate the optical properties, which agree well with the experimental results.

Keywords: liquid crystals; orientational transition; birefringence; FDTD

#### 1. Introduction

A variety of induced orientational transitions of liquid crystals (LCs) have been extensively investigated since the mesophase material was discovered. The birefringence comes from the orientation of anisotropic LC molecules with respect to the polarisation direction of incident light. The birefringence of LCs can be induced by temperature, surface anchoring condition, pressure, electrical and magnetic fields [1-6]. External electric field-driven orientational transition has been used in many applications, such as LC displays and optical modulators. Recently, surface-induced orientational changes in LC films have proven to be highly effective in amplifying the presence of targeted analytes in chemical and biological sensors. In the work of Abbott and Shah [3], a homeotropic alignment will change to homogeneous in detecting part-per-billion concentration of dimethymethyphosphonate (DMMP). With the advance of micro- and nano-fabrication techniques, orientational transitions in microtextured substrates have been studied [4, 5]. In this work, we demonstrate induced orientational transition of LC E7 between two optical fibre tips in a gravitational field as a result of minimising the free energy. The transition is from a homeotropic state with respect to the fibre tip, which has no birefringence effects on propagated light, to a tilted state, which makes differently polarised light propagate at different speeds. We establish a model based on the competition between the Frank-Oseen elastic energy and the gravitational potential energy to explain the origin of the observed transition. At short spacing, the undistorted

homeotropic orientation of LC is preferred; however, at longer spacing, a distorted orientation is preferred. The orientational distortion introduces birefringence in the optical fibre, which changes the polarised direction of output light. Once the LC director profile is known, the Finite Difference Time Domain (FDTD) code, written in Matlab, is used to calculate the optical properties.

### 2. Experimental details

The experiment was performed on an optical fibre alignment stage (Newport) with a movement resolution 0.05 µm as shown in Figure 1(a). A 632.8 nm polarised He-Ne laser (Melles Griot) was coupled into the optical fibre (Corning SMF-28). The fibre is cylindrical with a 125 um diameter cladding and an 8.2 µm diameter core. The outer buffer coating on the optical fibre was removed using a stripper, and the fibre tip was cleaved perpendicularly to obtain a flat end face. The polarisation direction was around 45° with vertical direction. Before the output light reached an optical power detector (Newport), an analyser parallel to the original polarisation direction was added in order to analyse the polarisation direction of output light due to the birefringence introduced by distorted LC (Figure 1(d)). In order to obtain homeotropic alignment on fibre tips, the fibre tips were dipped into a polymaleic anhydride solution in toluene with concentration 4% w/w. The fibres were shaken to remove surplus solution, and dried at room temperature for 30 min. Two fibre tips were aligned to have

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Figure 1. (a) Experimental setup (optical fibre alignment stage). (b) Photograph of liquid crystal (LC) between fibre tips at about 150  $\mu$ m spacing (top view). The scale bar is 50  $\mu$ m. (c) Photograph of LC between fibre tips at about 100  $\mu$ m spacing (top view). The scale bar is 50  $\mu$ m. (d) Schematic of LC between two optical fibre core tips.

maximum output power coaxially. The spacing between fibres was then set to  $150 \,\mu\text{m}$ . A small amount (about 0.1  $\mu$ L) of E7 LC (EM Industries) was applied between two fibre tips, as shown in Figure 1(b). For the long spacing, the cross-section of LC matches well with that of the fibre, as shown in Figure 1(b). For the short spacing, the cross-section of LC was increased, as shown in Figure 1(c).

The experimental results are shown in Figure (2). When the scan in the axial direction of fibre was from  $30 \,\mu\text{m}$  to  $150 \,\mu\text{m}$  at a speed of  $50 \,\text{nm s}^{-1}$ , the first valley occurred at about 65 µm. Scanning from 150 µm to  $30 \,\mu\text{m}$  at a speed of  $50 \,\text{nm s}^{-1}$ , the last valley occurred at around 75 µm. The dynamic response of the LC could explain the difference. We hypothesise that gravity, like an external electric or magnetic field, gives a fast and easy switch-on and a slow and rigid switch-off. The induced transition is from a more ordered state to a less ordered state when the spacing is increased. These valleys indicate that the phase difference of the polarised light in y and z direction is a multiple of  $\pi$ . If there is no orientational transition of the LC, there is no phase difference and the optical power should decrease monotonously. Since the diameter of the fibre core is much smaller than the diameter of the LC cross-section, and the transition occurs at a short spacing where the strong anchoring at the fibre tip surface dominates the anchoring at the LC-air interface, the orientation at the LC-air interface has negligible effect on the centre of the LC (between the fibre core).



Figure 2. Output optical power depends on the distance between two fibre tips.

#### 3. Theoretical model

In the small fibre core area where the strong anchoring at the fibre tip surface is dominant at a short spacing, it is assumed that the distortion of the LC director far from the LC–air interface is uniform in the y and z directions. Consider a nematic LC sample suspended between two optical fibre core tips with a distance lapart, as shown in Figure 3.

The director on the fibre tips is strongly anchored so that the director n is  $\vec{n} = (\cos \theta, 0, \sin \theta) = (1, 0, 0)$ with  $\theta = 0$  at x = 0, *l*.  $\Theta$  is the tilted angle and *l* is the



Figure 3. (a) Illustration of liquid crystal (LC) director on a short spacing. (b) Illustration of LC director on a long spacing. (c) Coordinate for the LC distortion on the influence of gravitational field.

spacing distance. For simplicity, one elastic constant approximation is used. Using index notation and the Einstein summation, the Frank–Oseen elastic energy density  $w_f$  is

$$w_f = \frac{1}{2} K n_{i,j} n_{i,j} = \frac{1}{2} K \theta'^2, \qquad (1)$$

where *K* is the elastic constant of the LC, *i*, *j*, and *k* are the indices of coordinate, and comma denotes a partial derivative. The gravitational potential energy density  $w_g$  is

$$w_g = \rho g h, \tag{2}$$

where  $\rho$  is the mass density of the LC, g is the gravitational constant and h is the height of the LC. From the symmetry of the LC distortion, we can expect symmetric solution

$$\theta(x) = \theta(l - x), \tag{3}$$

satisfying  $\theta'(\frac{l}{2}) = 0$ . The undistorted solution is  $\theta(x) = 0, h(x) = 0$ . The total free energy is zero. Now we seek the solution in the form

$$h(x) = \frac{a}{2} \left[ \cos\left(\frac{2\pi}{l}x\right) - 1 \right],\tag{4}$$

satisfying h(0) = 0 and  $h(\frac{1}{2}) = -a$ . Then the tangent of the tilted angle  $\theta$  can be expressed by

$$\tan(\theta) = h'(x) \quad \text{with} \quad h'(x) = -\frac{a\pi}{l} \sin\left(\frac{2\pi}{l}x\right).$$
(5)

This leads to

$$\theta = \tan^{-1} \left[ -\frac{a\pi}{l} \sin\left(\frac{2\pi}{l}x\right) \right] \text{ and} \theta' = \frac{-\frac{2a\pi^2}{l^2} \cos\left(\frac{2\pi}{l}x\right)}{1 + \left[ -\frac{a\pi}{l} \sin\left(\frac{2\pi}{l}x\right) \right]^2}.$$
 (6)

Now the total energy per unit area of the LC sample is

$$W = \int_{0}^{l} (w_f + w_g) dx$$
$$= \int_{0}^{l} \left\{ \frac{1}{2} K \left\{ \frac{-\frac{2a\pi^2}{l^2} \cos\left(\frac{2\pi}{l}x\right)}{1 + \left[-\frac{a\pi}{l} \sin\left(\frac{2\pi}{l}x\right)\right]^2} \right\}^2 \right\} dx.$$
$$+\rho g \frac{a}{2} \left[ \cos\left(\frac{2\pi}{l}x\right) - 1 \right]$$

To demonstrate that the total energy of the distorted solution is smaller than that of the undistorted solution at longer distance, we take a = 0.2l, the mass density of LC sample  $\rho = 1020 kg/m^3$ , gravitational constant g = 9.8N/m, and elastic constant K =  $13.5 \times 10^{-12}$ N. The calculated results are shown in Figure 4. At a range of short distance, the elastic energy decreases dramatically. The gravitational energy decreases more slowly than the elastic energy. The total energy is below zero at a distance of about 43 µm, which means that the distorted director profile is preferred to the undistorted one. In the first approximation the surface energy variation is neglected. In further studies, the surface energy variation and its influence on the bulk LC should be included. The isotropic part of the surface energy of LC can be given approximately by  $F_s = \rho v^2 a$ , where  $\rho$  is the mass density, v is the velocity of sound and a is the molecular size [7]. So the surface energy is around  $10^{-1}$  J/m<sup>2</sup>. In the case of LC on fibre tips with a radius r, the surface area is  $S = 2\pi r l = 6.28 \times 10^{-4} \times 10^{-4} \approx 10^{-8} m^2$ . The total surface energy of the isotropic part is around  $F_s S \approx 10^{-9}$  J. The sum of elastic and gravitational energy is  $W\pi r^2 \approx 10^{-6} \times 3.14 \times (10^{-4})^2 \approx 10^{-14}$  J. The anisotropic part of the surface energy depends on the orientation of LCs at the interface. Thus, the surface energy change depends on the surface area and the orientation of the LC director at the LC-air interface. Furthermore, the size of the fibre core is much smaller than the crosssection of the LC, which means that the distance from the LC-air surface to the core is much larger than the coherent distance of the LC, and the influence of the surface at the fibre tip on the bulk LC orientation dominates.



Figure 4. Calculated free energy of liquid crystal between optical fibre tips.

Therefore, the change of surface energy due to the area change could be dominant over the change of elastic energy due to LC director distortion at the LC–air interface.

The distorted solution introduces birefringence when the light propagates. The propagation of the light wave depends on the LC director orientation and the direction of its polarisation. The FDTD method can be used to analyse the optical properties in this inhomogeneous and anisotropic medium. Maxwell's equations are solved directly in both space and time domains. We wrote the FDTD code in Matlab to simulate the optical properties of the LC between two fibre tips. The profile of LC director is given by Equation (6). The LC is E7 with the ordinary and extraordinary refractive indices  $n_o = 1.52$  and  $n_e = 1.74$  at wavelength  $\lambda = 633$  nm. For aligned E7 LC at wavelength  $\lambda = 633$  nm the scattering coefficient



Figure 5. Finite Difference Time Domain simulation results of light propagation through liquid crystal between optical fibre tips.

is around 4.2 cm<sup>-1</sup> at room temperature [8]. The results calculated by FDTD are shown in Figure 5. If there is no LC director distortion, the transmitted light through LC should obey the Beer-Lambert law  $I = I_0 e^{-(\alpha + \beta)}$ , where I and  $I_0$  are intensity of transmitted and incident light, respectively, and  $\beta$  and  $\alpha$ are absorption and scattering coefficients, respectively.  $\beta$  is negligible for LC. Thus, the detected light should be decreased exponentially and monotonously. If the distorted solution is preferred at short distance, the first valley would appear at around 10 µm. If the distorted solution is preferred at around 43 µm as calculated above, the first valley would appear at around 53 µm. Thus, the theoretical model explains well the origin of the observed orientational transition that comes from the competition between the Frank-Oseen elastic energy and the gravitational potential energy. At a spacing shorter than 43 µm, the undistorted homeotropic orientation of LC is preferred. However, at a spacing longer than 43 µm, a distorted orientation is preferred. This threshold effect of gravity is like the Frederiks threshold of electric or magnetic field in which LC begins to distort.

#### 4. Discussion

The observed orientational transition and birefringence may be useful for monitoring anchoring energy. In the case of weak anchoring, it is expected that the transition occurs at relatively shorter spacing, at which the transition cannot happen in the case of strong anchoring. Furthermore, monitoring the gravitationally induced birefringence may be a promising method to improve sensitivity in LC-based chemical and biological sensors [9, 10], with the advantages of optical fibre.

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