Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

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To cite this Article Vicari, L.(1999) 'Twist molecular orientation transition in a nematic liquid crystal cell', Liquid Crystals, 26: 12, 1837 — 1840

To link to this Article: DOI: 10.1080/026782999203490

URL: http://dx.doi.org/10.1080/026782999203490

LIQUID CRYSTALS, 1999, VOL. 26, NO. 12, 1837–1840

Preliminary communication

Twist molecular orientation transition in a nematic liquid crystal cell

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(*Received 16 March 1999; accepted 20 July 1999*)

We theoretically demonstrate that the application of a transverse next-to-static electric field to a planar nematic liquid crystal cell—obtained by strong planar anchoring of the liquid crystal on the first surface and negligible interaction with the second surface—causes an electro-reorientational transition of the Fréedericksz kind. We show that, above the transition the cell behaves as a twisted nematic liquid crystal cell with total twist depending on the applied voltage. Preliminary experimental results confirming the predicted effect are presented.

A common planar nematic liquid crystal cell is obtained by strong surface treatment of the cell walls in order to keep the molecular crystal director orientation parallel to the surfaces. The bulk orientation follows. When a low frequency electric field is applied transversely to this device, the molecular director is reoriented: the reorientation happens only if the applied electric field is higher than the Fréedericksz threshold [1]

$$E_{\mathrm{F}} = \left(\frac{4\pi^3 K_2}{d^2\,\Delta\varepsilon}\right)^{1/2}$$

and this reaches its highest value in the middle of the cell. Weak anchoring on both surfaces, resulting in a lowering of the threshold has been recently discussed [2]. Weak anchoring has been shown to expand the cell gap margin of a liquid crystal display operating by the in plane-switching mode.

A planar nematic liquid crystal cell can also be obtained by strong planar anchoring of the liquid crystal on the first surface and negligible interaction with the second surface. Owing to the presence of the free surface, the Fréedericksz threshold could be believed to disappear. In this letter we demonstrate theoretically, for the first time to our knowledge, that even in this case the application of a transverse next-to-static electric field generates an electro-reorientational transition of the Fréedericksz kind. Moreover, above the transition the cell behaves as a twisted nematic liquid crystal cell with a total twist depending on the applied voltage. Therefore, owing to the usual adiabatic rotation of light polarization by these cells, it can be used as a voltage-controlled light polarization rotator. Inserted between crossed or parallel polarizers, in a configuration similar to that of liquid crystal displays using a transverse applied electric field and now commercially available, it acts as an electrically controlled light valve controlling the pixel intensity with continuity from opaque to transparent states. Growing interest has recently been concentrated on this kind of device for commercial reasons: in fact they are considered as the basis of the next generation of liquid crystals displays [3]. Finally we observe that, for material characterization purposes, the proposed configuration can be used for the measurement of some properties of liquid crystals. Our theoretical predictions are confirmed by first experimental results.

The elastic free energy density f_{E} of a nematic liquid crystal can be written [4]:

$$f_{\mathrm{E}} = \frac{1}{2}\left[K_1\ \ (\mathrm{div}\,\mathbf{n})^2 + K_2\ \ (\mathbf{n}\ \ \mathrm{rot}\,\mathbf{n})^2 + K_3\ \ (\mathbf{n}\times\mathrm{rot}\,\mathbf{n})^2\right]$$

where K_i $(i = 1, 2, 3)$ are the Frank constants and $\mathbf{n}$ is the molecular director. In our frame, the two boundary planes are represented by $z = 0$ and $z = d$ where d is the cell thickness. Chemical and mechanical treatment are assumed at the $z = 0$ plane in order to obtain strong anchoring and planar alignment with the molecular director parallel to the x axis. We assume the nematic–substrate interaction at the $z = d$ plane to be negligible. We consider a uniform quasi-static electric field applied along the y axis. Since we do not have 'splay' or 'bend' solicitations, the first and third term in the elastic free

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energy density f_E can be disregarded and we have:

$$f_E = \frac{1}{2} K_2 (\mathbf{n} \quad \text{rot}\ \mathbf{n})^2$$

where only the 'twist' effect is taken into account. The molecular director is expressed by:

$$\mathbf{n} = \mathbf{x} \quad \cos \varphi(z) + \mathbf{y} \quad \sin \varphi(z)$$

where $\varphi(z)$ is the angle between the molecular director and the x axis at the depth z. Hence:

$$f_E = \frac{1}{2} K_2 \varphi_z^2$$

with

$$\varphi_z = \frac{\partial \varphi}{\partial z}.$$

In the absence of an electric field, the total free energy f is equal to the elastic free energy. It has a minimum for

$$\varphi_z = 0$$

so that the bulk is not deformed. Molecular orientation is determined by the strong anchoring condition on the first surface [5]:

$$\varphi(0) = \varphi(z) = \varphi(d) = 0.$$

When an electric field $\mathbf{E}$ is applied along the y axis, an additional term f_V has to be considered in the total free energy density. Since it holds [6] that

$$f_V = -\frac{\Delta\varepsilon}{8\pi} (\mathbf{n} \quad \mathbf{E})^2$$

where $\Delta\varepsilon$ is the dielectric anisotropy of the liquid crystal, for the total free energy density f we have:

$$f = f_E + f_V = \frac{1}{2} K_2 \varphi_z^2 - \frac{\mathbf{E}^2}{8\pi} \Delta\varepsilon \sin^2 \varphi. \tag{1}$$

It can be shown in general that, when f does not depend explicitly on z, it holds that:

$$\varphi_z \frac{\partial f}{\partial \varphi_z} - f = c^2$$

where c^2 is a constant. In our case this leads to:

$$K_2 \varphi_z^2 + \frac{\mathbf{E}^2}{4\pi} \Delta\varepsilon \sin^2 \varphi = c^2. \tag{2}$$

Imposing the natural boundary condition on the second cell wall

$$\varphi_z(d) = 0$$

we have

$$c^2 = \frac{\mathbf{E}^2}{4\pi} \Delta\varepsilon \sin^2 \varphi(d).$$

Substitution into equation (2) gives

$$\frac{4\pi K_2}{\mathbf{E}^2 \Delta\varepsilon [\sin^2 \varphi(d) - \sin^2 \varphi(z)]} \varphi_z^2 = 1$$

or

$$\frac{2}{\mathbf{E}} \left\{ \frac{\pi K_2}{\Delta\varepsilon [\sin^2 \varphi(d) - \sin^2 \varphi(z)]} \right\}^{1/2} \mathrm{d}\varphi = \mathrm{d}z. \tag{3}$$

Integrating we get

$$\frac{2}{E} \left(\frac{\pi K_2}{\Delta\varepsilon} \right)^{1/2} F\left[\frac{\pi}{2}, \sin^2 \varphi(d) \right] = d \tag{4}$$

where $F(\theta, x)$ denotes an elliptic integral of the first type that here is complete. Rearranging to

$$\frac{2}{d} \left(\frac{\pi K_2}{\Delta\varepsilon} \right)^{1/2} F\left[\frac{\pi}{2}, \sin^2 \varphi(d) \right] = \mathbf{E}$$

and observing that F is a function monotonically increasing from its minimum value $F(\pi/2, 0) = \pi/2$, we see that φ is unperturbed under a threshold value $\mathbf{E}_t$ given by

$$\mathbf{E}_t = \left(\frac{\pi^2 K_2}{d^2 \Delta\varepsilon} \right)^{1/2}. \tag{5}$$

This is similar to the usual critical field for the Fréedericksz transition. The threshold value is simply one half of that resulting from strong anchoring. In other words, when we realize negligible anchoring on a surface, we obtain the same threshold lowering that we would have by doubling the film thickness. Above $\mathbf{E}_t$ the maximum director rotation $\varphi(d)$ can be computed from equation (4). In figure 1 we report the results of this computation for a $d = 10\,\mu\text{m}$ thickness cell filled with a liquid crystal with $\Delta\varepsilon = 12$. As a parameter we use K_2 varying from 1 to 6 pN from left to right.

To verify that the molecular rotation is continuous and slow enough to guarantee the adiabatic rotation conditions [7], we have to calculate the molecular rotation angle versus z. Since now we know $\varphi(d)$, with this aim we can integrate equation (3) again from 0 to z, getting:

$$\frac{2}{\mathbf{E} \sin \varphi(d)} \left(\frac{\pi K_2}{\Delta\varepsilon} \right)^{1/2} F[\varphi(z), 1/\sin^2 \varphi(d)] = z$$

where the symbols have the same meaning as before. Now $\varphi(z)$ can easily be computed by standard numerical recipes. The results are shown in figure 2. We have set $d = 10\,\mu\text{m}$, $\Delta\varepsilon = 12$ and $K_2 = 3$ pN. Now we use as a

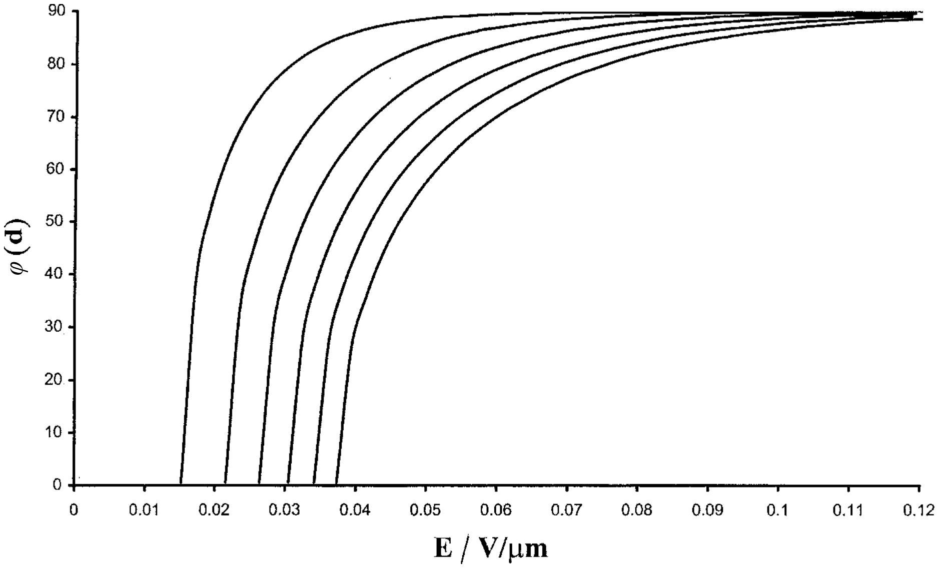

Figure 1. Maximum director rotation versus the applied electric field. As a parameter we use K_2 varying from 1 to 6 pN from left to right curve.

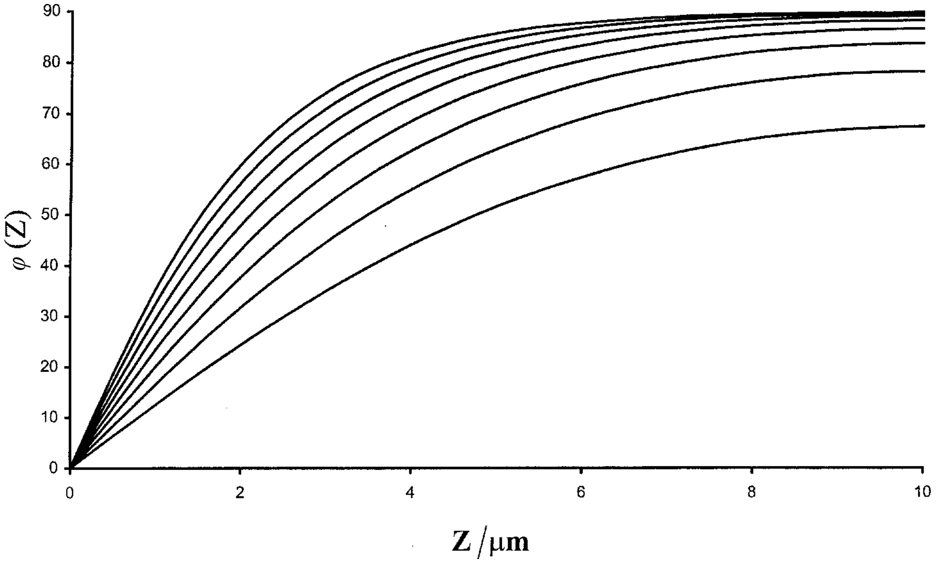

Figure 2. Molecular rotation angle versus z. From left to right curve, $\mathbf{E} = 0.11$; 0.10; 0.09; 0.08; 0.07; 0.06; 0.05; 0.04 V μm^{-1}, respectively.

parameter the applied electric field that is assumed to decrease from 0.11 to 0.04 V μm^{-1} from left to right, in steps of 0.01 V μm^{-1}. Since these values are quite typical for usual liquid crystals, we can see that the rotation length is longer than the typical wavelength ($\lambda = 0.5$ μm) even when a 90° rotation is generated. The hypothesis of adiabatic polarization rotation appears to be reasonable.

Despite the conceptual simplicity of the device, its experimental realization is not trivial. To our knowledge, a surface treatment able to eliminate chemical interaction between the liquid crystal and the glass is not available. As the 'free' surface we used clean glass. Chemical interaction of a liquid crystal and glass tends to be planar. However, in the absence of surface treatment and rubbing, no privileged direction is present except for that due to the layer absorbed by the surface which assumes a planar alignment oriented along the direction followed by the liquid crystal during cell filling. We used conducting spacers for the lateral confinement and for the application of the electric field. To lower the geometrical perturbation we used thin spacers ($d \approx 12$ μm) set far apart (≈ 700 μm), while to lower the chemical interaction we used a plastic film; this was aluminized in order to apply the electric field. As in our previous

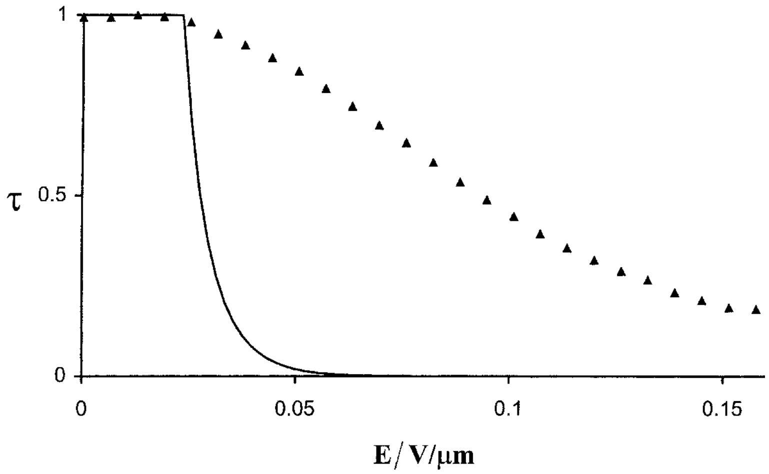

Figure 3. Sample transparency. Comparison between theoretical predictions (solid line) and experimental results (triangles).

work [8], for the planar surface we used a dichroic polarizer with rubbing treatment. The cell was filled by capillarity and a weak planar orientation induced on the 'free' surface. The liquid crystal used was 5CB (K15) (Merck UK, Ltd). We inserted the cell between parallel polarizers and detected with a photodiode the intensity of a HeNe laser beam passing through the sample. When the voltage was applied, by amplification of the signal from a pulse generator at a frequency of 1 kHz, the beam polarization was rotated by the cell and absorbed by the second polarizer.

In figure 3 we show the sample transparency τ computed by the theory presented (solid line) and compared with the experimental results (triangles). The expected threshold effect is clearly shown. The experimental decrease of transmitted light with increasing applied electric as described by the theory is sharper than the experimental decrease. We attribute this descrepancy to the fact that in the experiment interaction at the second interface cannot be completely disregarded.

In conclusion, we have theoretically predicted and experimentally shown the existence of a Fréedericksz type molecular orientation transition in a planar liquid crystal cell, with strong anchoring at the first surface and weak interactions at the second surface. Moreover we have shown the possibility of achieving a twisted nematic liquid crystal cell with total twist angle controlled by an applied voltage. The device can be used for the realization of low cost light polarization rotators, light valves and LCDs. From a fundamental point of view, the configuration examined can be useful as a method for measuring liquid crystal properties such as the K_2 Frank elastic constant for $\Delta\varepsilon$ and its dependence on the frequency of the applied voltage. Further work is required in order to find a surface treatment able to reduce the chemical interaction with the glass.

This work has been partially supported by MURST (PRIN 97).

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