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# Nematic director configurations in high pretilt, parallel aligned layers

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We describe the director configurations associated with a negative dielectric anisotropy, high pretilt (typically  $\sim 85^\circ$ ) nematic cell. A number of distinct director configurations are observed, with both a transition to a spontaneously twisted state and a nucleated transition mediated by disclination line movement. We discuss the role of surface pretilt and elastic constant anisotropy on behaviour and give results on the relative energetic stability of the director states.

## 1. Introduction

In recent years interest has grown in surface mode devices, a notable example being the pi-cell [1, 2] which utilizes two equal, low pretilt (typically  $1^\circ \sim 10^\circ$ ), parallel aligned surfaces and operates with the director in a bend configuration, maintained through application of a bias voltage,  $V_{\text{bias}}$  (typically  $\sim 2$  V), to a positive dielectric anisotropy nematic. If the applied voltage is modulated, but remains above  $V_{\text{bias}}$ , the director in the central region of the cell remains permanently aligned along the field direction, with director movement confined to the near-surface regions. The pi-cell can be readily made to exhibit combined 'on + off' electro-optic switching times of the order 5 ms and is thus an attractive mode for device consideration.

In this paper we describe an alternative effect utilizing high pretilt (typically  $\sim 85^\circ$ ) surfaces and negative  $\Delta\epsilon$  materials, allowing for the construction of a splayed, birefringent device. Some references to this arrangement occur in the literature [3–5], but we have not found a detailed discussion of the role of pretilt and elastic constant anisotropy on director behaviour.

## 2. Outline of physical behaviour

We observe three principal director configurations (figure 1) in high pretilt cells. Observations of these states made using the polarizing microscope for the negative dielectric anisotropy nematic ZLI-4788-000 (Merck UK) are shown in figure 2. In the absence of an applied voltage the high pretilt surfaces cause the LC to adopt a bend configuration (figure 1 a), shown extinguished between crossed polarizers in figure 2 (a). As shown in figure 1 b, application of low voltages (typically  $< \sim 1$  V)

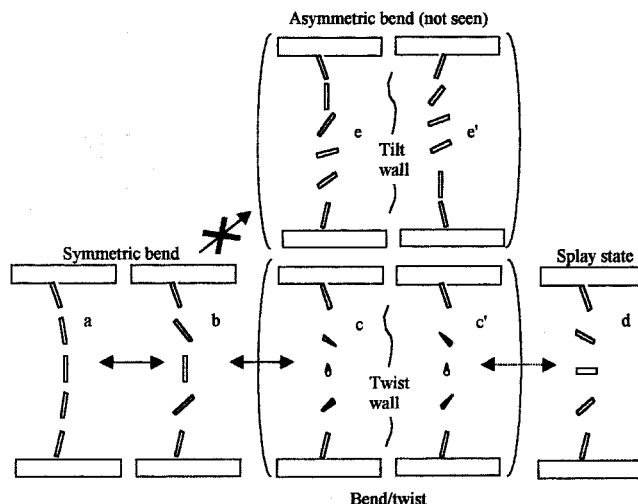


Figure 1. Director configurations associated with a high pretilt, negative  $\Delta\epsilon$  device.

causes a small symmetrical distortion of the bend state (accompanied experimentally by a small, thresholdless variation of optical transmission when the cell rubbing direction lies at an angle to the polarizer axes) with the director at the cell centre remaining perpendicular to the cell surfaces (i.e.  $\theta = \pi/2$  at  $z = d/2$ ).

By consideration of the conventional low pretilt, anti-parallel aligned, Fréedericksz transition or the splay-state behaviour in the pi-cell, one might expect the symmetric bend state to become asymmetric (i.e.  $\theta = \pi/2$  moving off centre to  $z \neq d/2$ ) above a critical voltage. Since the  $\theta = \pi/2$  point would be equally likely to move in the direction of  $z$  increasing or decreasing (figure 1 e and e'), tilt walls would accompany this transition. An alternative transition of lower energy (at least for conventional elastic constants values—see discussion below) is

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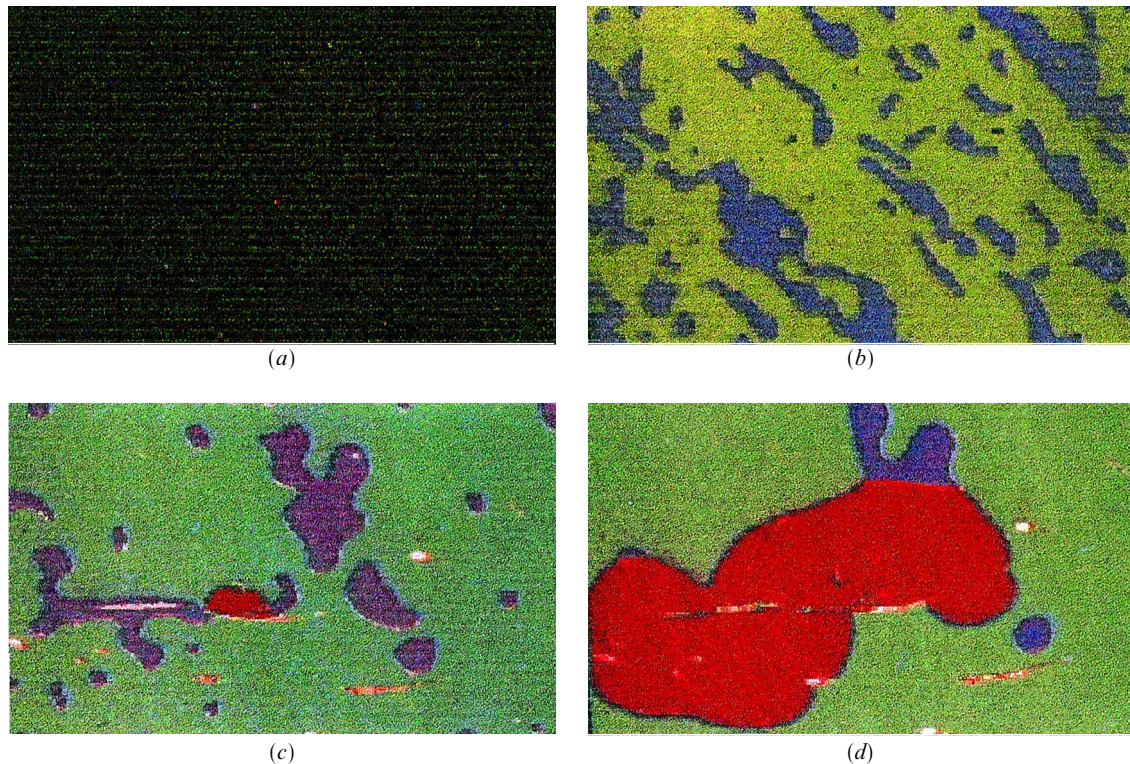


Figure 2. (Clockwise from top left,  $0.7 \times 0.5 \text{ mm}^2$  area of sample): (a) symmetric bend-state at 0 V extinguished between crossed polarizers; (b)  $\pm \pi$ -twist regions with accompanying twist walls at 3 V, polarizers uncrossed; (c) nucleation occurring on a surface scratch of the splay state (red) within majority  $\pm \pi$ -twist state; (d) growth of splay state.

possible however, with the director distorting in the plane perpendicular to the rubbing directions, adopting a  $\pi$ -twist. Naively this can be understood as being a consequence of the twist elastic constant,  $k_{22}$ , being of lower magnitude than the bend,  $k_{33}$ , (typically  $k_{11} \sim k_{33} \sim 2k_{22}$ ), so favouring twist deformations. The liquid crystal is not optically active and domains of both right and left handed twist form in equal amounts<sup>†</sup>, separated by twist walls (figure 1 c,c' and figure 2 (b)). The apparent spontaneous 'appearance' of twist is allowed, since at zero volts the twist is undefined at  $z = d/2$ , where the director reaches  $\theta = \pi/2$ .

As the voltage is increased further, the director tilt at the cell centre tends towards  $\theta = 0^\circ$ , with the majority of the ( $\pi$ ) twist confined to the near-surface regions. At high voltage the energy cost of confining the twist becomes large and we expect to see a transition to an untwisted splay state (figure 1 d). The situation is non-trivial however, since topology forbids a smooth and continuous transformation from the  $\pi$ -twist structure into the desired untwisted splayed state. Any such transition

<sup>†</sup> Experimentally, it is sometimes observed that with increasing voltage a slight predominance of one twist state occurs, which can be simply attributed to the two cell surfaces being very slightly non-parallel.

must be accompanied by the nucleation and movement of defects [6]. In real devices it is found that nucleation of the splay state often occurs on small inhomogeneities (dust particles, surface scratches, etc.), although details of the nucleation mechanism are not fully understood. Figure 2(c) shows the initial appearance of a splayed region (appearing red in the photo-micrograph) into the majority twist state (green/purple) with the subsequent growth of splayed regions, figure 2(d), via the movement of disclination lines, eventually filling the whole cell. The sample has been rotated slightly between the polarizers to image the splay state better in figures 2(c,d).

Once the splay state is established, modulation of the applied voltage causes a variation in optical transmission, with the director at the cell centre remaining perpendicular to the glass substrates and reorientation occurring in the near-surface regions. Measured relaxation speeds for a  $5.2 \mu\text{m}$ , ZLI-4788-00 cell in the splay state, switching from 8 V to 2 V, were of the order 10 ms at  $20^\circ\text{C}$ .

### 3. Energy considerations

We now consider the pretilt required to stabilize the zero-volt bend state shown in figure 1 a, for a given  $k_{11}/k_{33}$  ratio. Too low a surface pretilt favours a zero

volt splay state, required for a pi-cell. Solving the well known Frank free energy equation numerically (some analytic manipulation makes this a simple numerical task [7]) to find the 0 V director structure as a function of  $k_{33}/k_{11}$  gives the plot of figure 3. The logarithmic scale avoids the slight drawback of the linear plot (inset) of causing the (*a priori*) infinite number of materials with  $k_{11} < k_{33}$  to be confined between  $[0, 1)$  on the ordinate, obscuring the symmetry about the  $k_{11} = k_{33}$  point. In practice, most low molar mass materials have  $0.5 < k_{11}/k_{33} < 3$  and it is apparent that all pretilts above  $\sim 50^\circ$  stabilize the zero-volt bend state we require for this range.

For completeness we note that we have considered only 1D-splay and bend distortions in deriving figure 3. Both the pi-cell and current device possess regions of grad.  $n \neq 0$  at 0 V however (in contrast to the conventional anti-parallel aligned Fréedericksz cell), and so unusually large elastic constant anisotropy might lead to more complex director structures, possibly 2D-periodic structures [8] or spontaneously twisted states. We have not observed such structures in practice.

At low voltages the first threshold observed for the device is associated with tilting the director away from  $\theta = \pi/2$  at the cell centre. Figures 4 and 5 show, respectively, the tilt and twist profiles of an  $80^\circ$ -pretilt device with  $k_{11} = k_{33} = 2k_{22} = 10$  pN, and  $\Delta\epsilon = -5.7$ . Numerically, it is found that for voltages  $0 < V < 1.35$  V some small symmetric bend distortion occurs.

Above a voltage,  $V_\pi$ , ( $\approx 1.35$  V here) midplane tilt occurs (figure 6, solid line), perpendicular to the plane containing the surface rubbing directions, producing a  $\pi$ -twisted configuration. Constraining the tilt to lie within the rubbing plane gives the alternative threshold voltage,  $V_{As-Bend}$ , associated with the asymmetric bend

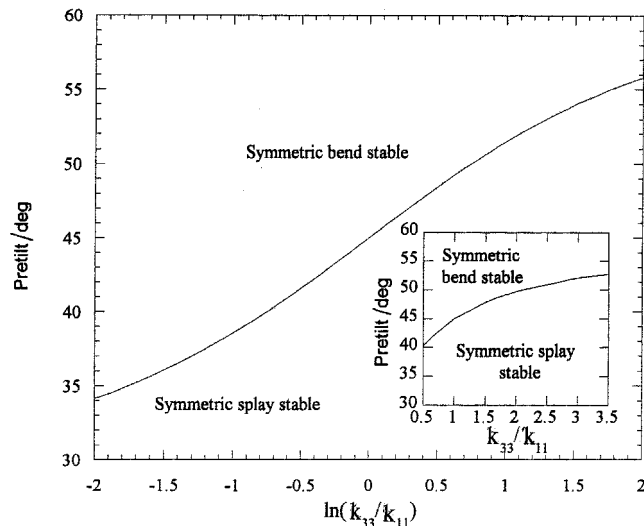


Figure 3. Stability diagram at 0 V.

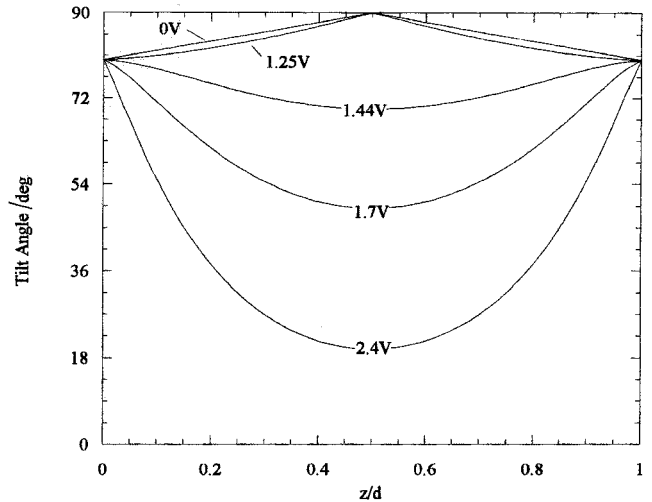


Figure 4. Variation of tilt angle with voltage:  $k_{11} = 2k_{22} = k_{33} = 10$  pN,  $\Delta\epsilon = -5.7$ , pretilt =  $80^\circ$ .

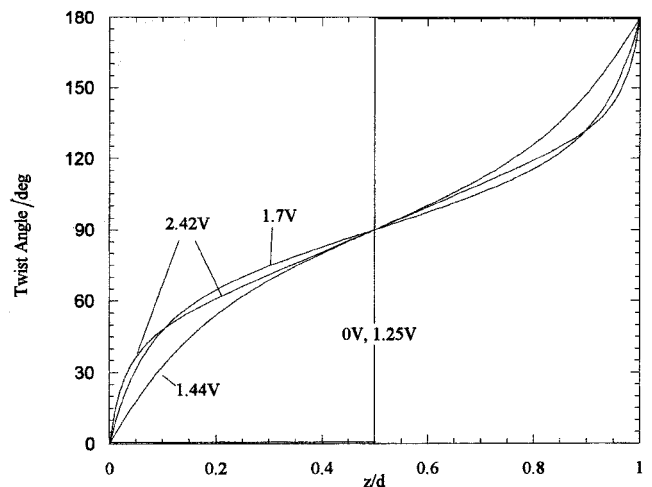


Figure 5. Variation of twist angle with voltage:  $k_{11} = 2k_{22} = k_{33} = 10$  pN,  $\Delta\epsilon = -5.7$ , pretilt =  $80^\circ$ .

state (figure 1 e,e') shown by the dashed line in figure 6. The  $\pi$ -twist configuration is seen to have a lower threshold voltage. Above  $V_\pi$  the subsequent appearance of the untwisted asymmetric bend state is topologically forbidden without a nucleated transition. The effect of pretilt on  $V_\pi$  and  $V_{As-Bend}$  is shown in figure 7. As the surface pretilt tends towards  $90^\circ$  we expect  $V_\pi$  and  $V_{As-Bend}$  to converge to the value for the homeotropic Fréedericksz threshold voltage,  $V_{Fréedericksz} = \pi(k_{33}/\epsilon_0 \Delta\epsilon)^{1/2}$  ( $\approx 1.4$  V for  $\Delta\epsilon = -5.7$  and  $k_{11} = k_{33} = 2k_{22} = 10$  pN).

In principle, for sufficiently large values of  $k_{22}/k_{33}$  one might expect  $V_\pi > V_{As-Bend}$ . Plotting the value of the threshold voltage  $V_\pi$  against  $k_{22}$ , keeping  $k_{11} = k_{33} = 10$  pN constant, and extrapolating, we find  $V_\pi = V_{As-Bend}$  for  $k_{22} \sim 35$  pN. We are not aware of any materials showing such extreme  $k_{22}/k_{33}$  anisotropy [9].

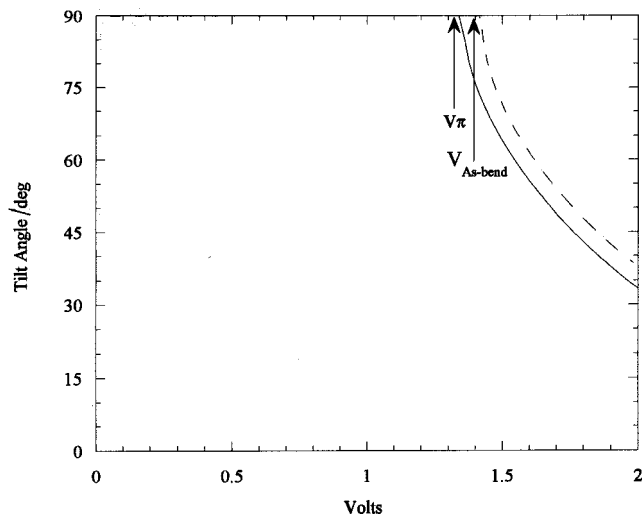


Figure 6. Threshold voltages for onset of  $\pi$ -twist ( $V_\pi$ ) and asymmetric bend ( $V_{As-bend}$ ) states.

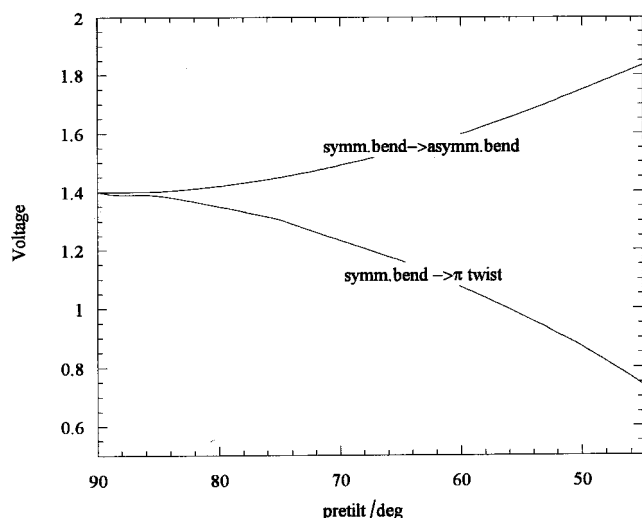


Figure 7. Threshold voltage behaviour vs. pretilt ( $k_{11} = 2k_{22} = k_{33} = 10$  pN,  $\Delta\epsilon = -5.7$ ).

We now consider the transition from the  $\pi$ -twist state (figure 1c,c') to the symmetric splay state (figure 1d). These director configurations are metastable with respect to one another and any transition necessarily involves the nucleation of defects. Figure 8 shows a plot of Gibbs energy against voltage for a number of the states shown in figure 2. We again take  $k_{11} = k_{33} = 2k_{22} = 10$  pN and pretilt =  $80^\circ$ . The four lines b, c, d, e, respectively, correspond to the symmetric bend state (figure 1a,b), the  $\pi$ -twist (figure 1c,c'), the splay state (figure 1d) and an asymmetric bend state (figure 1e,e') (not seen in practice, see above). With the chosen scaling of the axes, the points of intersection of the lines b, c and e are not clear, but figure 6 showed the transition to the  $\pi$ -twist state to occur at  $V_\pi \approx 1.35$  V. From figure 8 it is apparent that

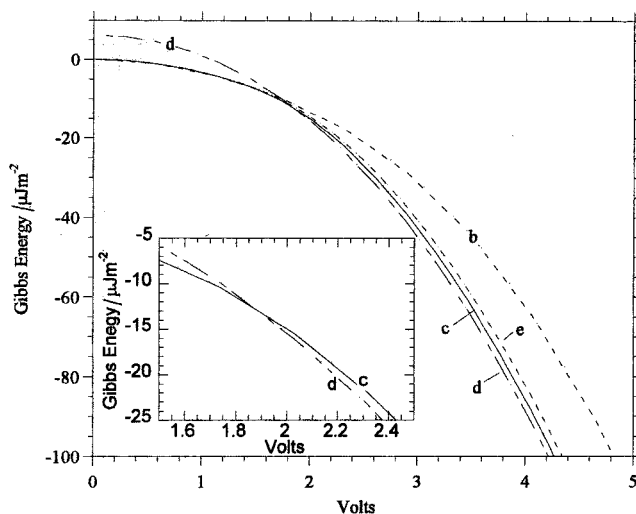


Figure 8. Variation of Gibbs free energy with voltage for states shown in figure 1.

once established, the  $\pi$ -twist state remains of lower energy than either the symmetric or asymmetric bend for all higher voltages. Above  $\sim 1.9$  V the splay state becomes the state of lowest energy (see inset, figure 8), and assuming that an appropriate nucleation site exists in a cell we can expect this state to form.

To summarise, figure 9 shows the pretilt/voltage phase diagram of the states found for a device with  $\Delta\epsilon = -5.7$  and  $k_{11} = k_{33} = 2k_{22} = 10$  pN. Below  $45^\circ$  a conventional (splayed) pi-cell forms at low voltage (c.f. figure 3).

#### 4. Conclusion

Application of voltage to a negative dielectric anisotropy nematic, confined between high pretilt parallel aligned surfaces, results in a complex display of director

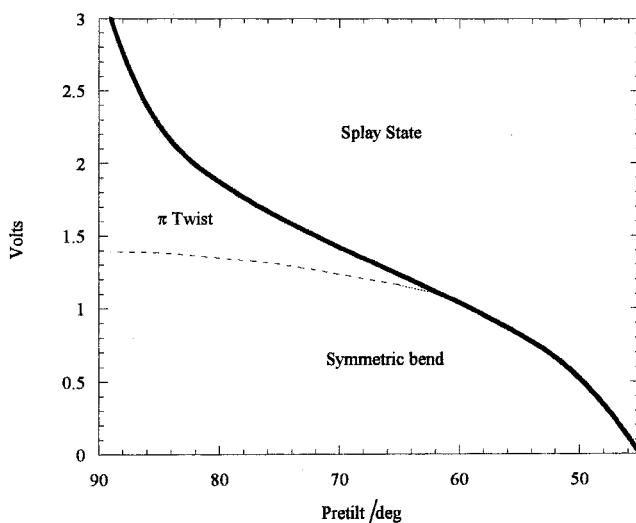


Figure 9. Phase diagram of states ( $k_{11} = 2k_{22} = k_{33} = 10$  pN,  $\Delta\epsilon = -5.7$ ).

reordering, including spontaneous symmetry breaking, the appearance of twist and a defect-mediated (nucleated) transition.

A pretilt/voltage phase diagram of director states has been calculated. At 0 V all pretilts above  $\sim 50^\circ$  are found sufficient to stabilize a uniform bend state for  $k_{33}/k_{11}$  in the range common to most nematics (typically,  $0.5 < k_{33}/k_{11} < 3$ ).

Energy calculations suggest that asymmetric bend states, analogous to the asymmetric splay states of low pretilt Fréedericksz and pi-cells, do not appear for realistic values of elastic constants, with instead director reorientation proceeding via a  $\pm \pi$ -twist configuration.

Even in the absence of applied voltage, the bend-director configuration results in a finite elastic energy density. We suggest that it may be of future interest to examine the possibility that highly anisotropic elastic constant ratios, such as may be obtained in some polymeric systems, may lead to more complex 0 V director configurations.

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- [9] THURSTON, R. N., and ALMGREN, F. J., 1981, *J. Physique*, **42**, 413. A condition is derived, namely  $(k_{11}/k_{33}) \geq 3(k_{22}/k_{33} - 1)$ , that a geodesic surface, which portrays equilibrium director configurations, exists for a nematic. We note that the stated elastic constants do not satisfy this condition, although we are unclear as to the physical significance of this result.