Flexoelectric Surface Switching of Bistable Nematic Devices

Colin Denniston[1] and J. M. Yeomans[2]

[1]*Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218*
[2]*Department of Physics, Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, England*

We report on a novel method of dynamically controlling the boundary conditions at the surface of a nematic liquid crystal using a surface flexoelectric effect. By moving the surface directors we show that one is able to manipulate defects which lie near the surface. This can be used to produce switching of a nematic liquid-crystal device between two states with very similar free energies. This results in a bistable device that can retain either state with *no* applied voltage. Switching between the states occurs when the movement of the surface directors rotates those in the bulk which are then able to create or annihilate defects which lie near the surface of the device.

Defect structures in liquid crystals naturally evoke interest due to the appearance of complex textures easily visible by the naked eye. Early studies focused on classifying the static properties of the defects and their interactions [1,2]. More recently the focus has moved to examining the dynamics of topological defects [3].

In most practical applications of liquid crystals, such as traditional display devices, defects destroy the optical properties and are undesirable. However, novel display designs, such as bistable displays or multidomain nematics, exploit defect properties. Most attempts to control the defect motion have made use of bulk electric fields [4]. In this Letter we will show how the flexoelectric effect can be used to control the surface alignment of a liquid crystal, thereby manipulating defects near the surface and switching the state of a liquid-crystal display device.

Liquid crystals are typically comprised of highly anisotropic, rod-shaped molecules. The nematic phase, which we shall concentrate on here, occurs when the molecules align parallel giving rise to long-range orientational order with the direction of alignment indicated by the so-called director field [2]. In a typical display device, the liquid crystal is confined between two plates a few microns apart. The director configuration on the plates is fixed. When an electric field is switched on, the molecules align in the direction preferred by the field. After switching off the field, long-range elastic interactions ensure that the molecules reorient themselves in the direction preferred by the surfaces. These devices can be used as displays because different liquid-crystal orientations have different optical properties. The switching of such traditional liquid-crystal devices is well understood.

However, there is now considerable interest in developing bistable devices which can retain a memory of two distinct states, with different liquid-crystal orientations, and, hence, different optical properties, even when the field is switched off [5,6]. It has been demonstrated, both by minimizing a Landau–de Gennes free energy functional and by experiments [5,7], that it is possible to produce two (meta)stable states with different orientations of the direc-

tor in the bulk by having different configurations of defects near the surface. However, the process of switching between these two states is not understood. As the switching involves changes in the configuration of the defects near the surface, controlling this process requires understanding the dynamics of defects and how they can be manipulated.

In this Letter we describe the physics behind the switching dynamics of a simple bistable nematic device. Our main conclusions are that the driving force which causes the switching is a surface flexoelectric effect. This rotates the surface directors which in turn pull around the bulk director field allowing the defects which lie near the surface of the device in one of the bistable configurations to be formed or annihilated. Once this is done, switching is essentially complete and the driving field can be removed.

The main barrier to understanding the dynamics of liquid crystals is the complexity of the liquid-crystal equations of motion. The hydrodynamics of liquid crystals are usually described by the Ericksen-Leslie-Parodi equations [2]. However, these are not sufficient to describe switching in bistable devices because they are restricted to an order parameter of constant magnitude. Defect motion, which plays a major role in the bistable switching, is not included.

Therefore it is necessary to consider a more general formalism of the hydrodynamics in terms of a tensor order parameter, $\mathbf{Q}$ [8]. $\mathbf{Q}$ evolves according to a convection-diffusion equation,

$$(\partial_t + \vec{u} \cdot \nabla)\mathbf{Q} - \mathbf{S}(\mathbf{W}, \mathbf{Q}) = \Gamma \mathbf{H}, \tag{1}$$

where $\vec{u}$ is the bulk fluid velocity and Γ is a collective rotational diffusion constant. The term on the right-hand side of Eq. (1) describes the relaxation of the order parameter towards the minimum of the free energy $\mathcal{F}$,

$$\mathbf{H} = -\frac{\delta \mathcal{F}}{\delta \mathbf{Q}} + (\mathbf{I}/3)\text{Tr}\left\{\frac{\delta \mathcal{F}}{\delta \mathbf{Q}}\right\}. \tag{2}$$

The order parameter distribution can be both rotated and stretched by flow gradients. This is described by the term on the left-hand side,

$$\mathbf{S}(\mathbf{W}, \mathbf{Q}) = (\xi \mathbf{D} + \mathbf{\Omega})(\mathbf{Q} + \mathbf{I}/3)$$
$$+ (\mathbf{Q} + \mathbf{I}/3)(\xi \mathbf{D} - \mathbf{\Omega})$$
$$- 2\xi(\mathbf{Q} + \mathbf{I}/3)\mathrm{Tr}(\mathbf{QW}), \qquad (3)$$

where $\mathbf{D} = (\mathbf{W} + \mathbf{W}^T)/2$ and $\mathbf{\Omega} = (\mathbf{W} - \mathbf{W}^T)/2$ are the symmetric part and the antisymmetric part, respectively, of the velocity gradient tensor $W_{\alpha\beta} = \partial_\beta u_\alpha$, and ξ is related to the aspect ratio of the molecules. The velocity field $\vec{u}$ obeys the continuity equation and a Navier-Stokes equation with a stress tensor generalized to describe the flow of liquid crystals. The details of the equations of motion can be found in Ref. [8]. We stress that the equations include backflow, allow variations in the magnitude of the order parameter, and follow the hydrodynamics of topological defects. To solve them, we use a recent lattice Boltzmann approach which is proving particularly robust for problems which relate to complex fluids [9].

We consider a liquid crystal described by the Landau–de-Gennes free energy [2],

$$\mathcal{F} = \int_V dV\{F_b - F_E + F_d\} + \int_{\partial V} dS\{F_a\}, \qquad (4)$$

where

$$F_b = \frac{A}{2}\left(1 - \frac{\gamma}{3}\right)Q_{\alpha\beta}^2 - \frac{A\gamma}{3}Q_{\alpha\beta}Q_{\beta\gamma}Q_{\gamma\alpha}$$
$$+ \frac{A\gamma}{4}(Q_{\alpha\beta}^2)^2,$$
$$F_E = \frac{\epsilon_a}{12\pi}E_\alpha Q_{\alpha\beta}E_\beta \qquad (5)$$
$$+ (\partial_\beta Q_{\alpha\beta})(\epsilon_{f_1}E_\alpha + \epsilon_{f_2}Q_{\alpha\gamma}E_\gamma),$$
$$F_d = \frac{\kappa}{2}(\partial_\alpha Q_{\beta\lambda})^2, \qquad F_a = \frac{\alpha_s}{2}(Q_{\alpha\beta} - Q_{\alpha\beta}^0)^2.$$

(Greek subscripts represent Cartesian directions and the usual summation over repeated indices is assumed.) The bulk free energy terms F_b describe a liquid crystal with a first-order, isotropic-nematic transition at $\gamma = 2.7$ [10]. Contributions to the free energy which arise from an imposed electric field $\vec{E}$ are included in F_E. Note that there are bulk terms which depend on $\mathbf{Q}$ and flexoelectric terms which couple to the derivatives of $\mathbf{Q}$ [11,12]. It is the latter that we shall focus on in this paper. They arise in liquid crystals where molecules are asymmetric in shape and carry a dipole moment. Alignment of the dipoles by a field can then lead to a varying director field being energetically favorable. F_d describes the elastic free energy within a one elastic constant approximation [2,13], and F_a is a surface free energy which fixes a preferred orientation $\mathbf{Q}^0$ for the surface director field [14].

We work in two dimensions and consider the geometry shown in Fig. 1. The device width is L_x and periodic boundary conditions are imposed in the y direction. The surface pinning potential at $x = 0$ is periodic with the director preferring to lie in the (x, y) plane at an angle
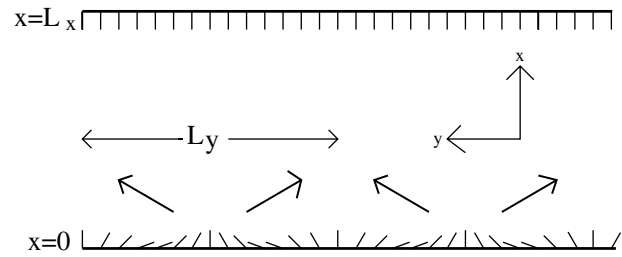

FIG. 1. The geometry used to demonstrate flexoelectric switching in a bistable nematic device. In particular, note the orientation of the director on the surfaces of the device. The bold arrows show the direction in which the surface directors rotate when a field is applied in the negative x direction.

$\theta_0 = (78\pi/180)\sin(2\pi y/L_y)$ to the x axis. At $x = L_x$ we take $\theta_0 = 7\pi/180$.

Our aim is to show that in a device of this geometry switching can be driven by a *surface* flexoelectric effect and to demonstrate the kinetic pathway along which the switching proceeds. Therefore we put ϵ_a and ϵ_{f2} in the free energy expression (5) equal to zero [15]. Integrating by parts shows that the remaining flexoelectric term can be rewritten as a surface contribution

$$\int_{\partial V} dS\{\sigma_\beta E_\alpha Q_{\alpha\beta}\}, \qquad (6)$$

where $\boldsymbol{\sigma}$ is the surface normal. In the geometry of Fig. 1, we will apply an electric field along x. Symmetry suggests, and we find in our simulations, that the director remains in the (x, y) plane. In this case, assuming uniaxiality [so that $Q_{xx} = q^2(\cos^2\theta - 1/3)$, where q is related to the largest eigenvalue of Q], and ignoring elastic and bulk contributions, the surface free energy density at $x = 0$ is

$$F_s = \frac{q^2\alpha_s}{2}(\theta - \theta_0)^2 + q^2\epsilon_{f_1}E_x(\cos^2\theta - 1/3), \quad (7)$$

where θ is the angle the director makes with the x axis. Minimizing with respect to θ gives, for small deviations,

$$\theta - \theta_0 = \epsilon_{f_1}E_x/\alpha_s \sin 2\theta. \qquad (8)$$

Switching will be driven by a series of voltage pulses:

$$V = 0, \qquad 0 < t < t_0, \qquad (9)$$
$$V = +V_0, \qquad t_0 < t < t_0 + t_1, \qquad (10)$$
$$V = 0, \qquad t_0 + t_1 < t < 2t_0 + t_1, \qquad (11)$$
$$V = -V_0, \qquad 2t_0 + t_1 < t < 2t_0 + 2t_1. \qquad (12)$$

The first voltage pulse corresponds to a field in the negative x direction. Then for $0 < \theta < \pi/2$, $\theta - \theta_0$ is negative; for $-\pi/2 < \theta < 0$, $\theta - \theta_0$ is positive. Therefore all the surface directors move towards the vertical as shown by the arrows in Fig. 1. This will tend to favor vertical alignment, with the director field parallel to the x axis, in the bulk. Conversely, a field in the positive x direction causes the directors to move away from $\theta = 0$ favoring a bulk state with the director field aligned diagonally as

a: t=2000   f: t=6000

b: t=2500   g: t=6100

c: t=2900   h: t=6300

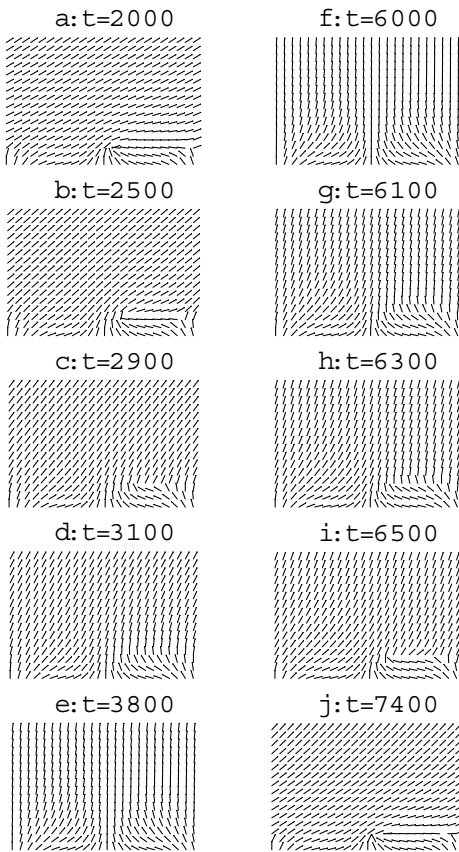d: t=3100   i: t=6500

e: t=3800   j: t=7400

FIG. 2. Snapshots of the director configuration during switching: (a) no field; (b)–(e) switching from diagonal to vertical; (f) no field; (g)–(j) switching from vertical to diagonal. Times are measured in simulation units.

FIG. 3. Variation of the total, elastic, and bulk free energies (measured relative to the total free energy with no applied field) with time t. A field along $-\vec{x}$ is switched on at $t_0 = 2000$ and off at $t_0 + t_1 = 4000$. A field along $+\vec{x}$ is switched on at $2t_0 + t_1 = 6000$ and off at $2t_0 + 2t_1 = 8000$. Times, measured in simulation units, are comparable in Figs. 2 and 3.

shown in Fig. 2a. Thus the surface flexoelectric term can provide a driving force for the switching.

Simulations of the full Eqs. (1)–(5) displayed in Fig. 2 show the path by which switching proceeds. At each time, we display that portion of the device which lies near the $x = 0$ surface. The voltage pulses cause the system to cycle between the states shown in Figs. 2a and 2f which are stable in the zero field portions of the voltage cycle [(9) and (11), respectively]. These have very similar free energies because of the imposed geometry. We find a free energy difference, measured as a fraction of the elastic energy, of 0.2%. The other frames in Fig. 2 show how the system moves between the bistable states. To switch from diagonal to vertical (Figs. 2a–2e), the surface deformation pulls the bulk directors towards the vertical. This provides the driving force for the pairs of defects at the surface to move together and annihilate. The switch from vertical to diagonal (Figs. 2f–2j) occurs in a similar way with the bulk rotating until there is sufficient driving force that the defects can be reformed.

Further insight into the process can be obtained by considering the free energy. This is shown in Fig. 3 where the bulk, elastic, and total (elastic + bulk + surface + flexoelectric) free energies are plotted as a function of time.
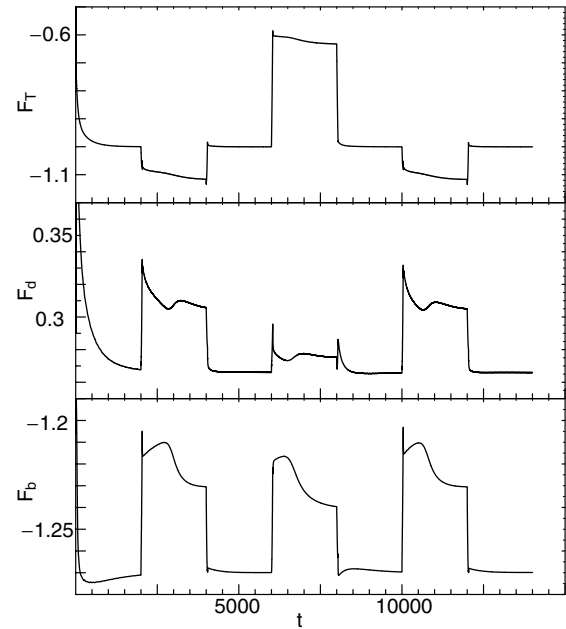
Upon switching the field, there is a small spike in the free energy which quickly relaxes as the surface directors move to their new positions. The switching itself is a far slower process—the elastic energy decreases slowly at the expense of the bulk free energy as the directors are pulled around by the surface until it is possible to push the defects out of or pull them into the device. Defect removal or creation is marked by a maximum in the elastic free energy, which becomes more pronounced as the switching time becomes longer, together with a faster decrease in the bulk free energy. Once the elastic free energy has passed this maximum, switching will occur if the field is removed.

The parameters used to obtain the results in Fig. 3 were, in simulation units, $A = 1.0$, $\Gamma = 0.5$, $\gamma = 3.0$, $\kappa = 2.0$, $\xi = 0.52$, $t_0 = 2000$, $t_1 = 2000$, $L_x = 63$, and $L_y = 24$. The dimensionless ratio $r \equiv \epsilon_{f1} E / \alpha_s = 0.21$ and the voltage was ramped up or down over 40 time steps. The simulation parameters can be mapped to physical values for comparison to prototype devices. However, the mapping must be treated with some caution because the simulations are in two dimensions. We choose length, time, and pressure scales so that $L_x = 1 \mu m$, pressure $= 10^5 \, N \, m^{-2}$, viscosities $\sim 0.04-0.1 \, Pa \cdot s$, $\kappa = 5 \times 10^{-11} \, N$, and switching times $\sim 10^{-4} \, s$.

r is a measure of the efficacy of the flexoelectric effect in rotating the surface directors. For a given device this ratio is controlled by the applied voltage. As expected, the switching time increases rapidly with decreasing r. As r decreases further switching fails. For example, for

$r = 0.05$ and $L_x = 63$, switching had not occurred after 10 ms. Moreover, there was no discernible variation of the free energy with time suggesting that switching would not occur at a later time.

It is also interesting to consider the effect of increasing L_x on switching times. The vertical to diagonal switching time is little changed by doubling the device width, whereas the diagonal to vertical switching time increases substantially. This is because an increase in L_x, without changing other parameters, favors the diagonal state over the vertical one: The difference in their free energies is now 5.8% of the elastic free energy.

As κ is decreased the switching time increases. This happens because the diffusion constant for the relaxation of the orientation of the director is proportional to κ. For small κ switching fails. This occurs when the elastic coupling between the surface and bulk directors becomes too small for the bulk to be rotated by a surface perturbation.

In the simulations it is possible to "turn off" backflow effects, that is, to ensure that any movement of the director field does not induce a flow. This has little effect upon the switching time. Increasing the temperature towards that of the nematic-isotropic transition leads to a decrease in switching time because the defects have a lower pinning energy.

The simple device described here has allowed us to obtain a fuller understanding of a possible switching mechanism in bistable displays. Experiments on prototype devices have reported switching times somewhat longer than those calculated here. One likely reason for this is that we have tuned the free energy of the two metastable states to be very nearly equal. As we saw when changing the device width, the switching time is strongly dependent on this free energy difference. Moreover, in a real liquid crystal, there will in general be a bulk field term in the free energy ($\epsilon_a \neq 0$). This may cause the switching in one direction to be due to a Frederiks' transition and inhibit switching in the other direction. A change in boundary conditions could be used to compensate for this imbalance. Other differences in prototype devices are that the modulated director structure at the surface is created using normal alignment on a blazed surface rather than modulated alignment on a flat surface. Work to incorporate this additional physics is currently underway.

In conclusion, we have shown that it is possible to model the switching mechanism in a bistable nematic device using lattice Boltzmann simulations of the liquid-crystal equations of motion. Thus we have been able to show that switching can be driven by a surface flexoelec-tric term in the free energy. Bistability occurs because the diagonal and vertical director alignments have very similar free energies. They remain stable because there is a free energy barrier between them. To promote switching, defects need to be introduced to or expelled from the device: This is most easily accomplished if the defect pinning energy is small.

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