Switching hydrodynamics in multi-domain, twisted nematic, liquid crystal devices

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Abstract. – We study the switching dynamics in two-domain and four-domain twisted nematic liquid crystal devices. The equilibrium configuration of these devices involves the coexistence of regions characterised by different handedness of the inherent director twist. At the boundaries between these regions there are typically disclinations lines. The dynamics of the disclination lines controls the properties, and in particular the switching speed, of the devices. We describe their motion using a numerical solution of the Beris-Edwards equations of liquid crystal hydrodynamics. Hence we are able to explain why a conventional two-domain device switches off slowly and to propose a device design which circumvents this problem. We also explain the patterns of disclination creation and annihilation that lead to switching in the four-domain twisted nematic device.

Introduction. – Twisted nematics (TN) are commonly employed in the construction of flat panel liquid crystal displays [1]. In a TN device, the equilibrium configuration is one in which the director field of the liquid crystal twists across the cell, normally because of conflicting homogeneous anchoring at the boundaries. Though traditional, single domain, TN devices can be built cheaply and easily, it is well known that they do not have ideal viewing angle properties [2]. To circumvent this, a number of possible solutions have been suggested. One partially successful avenue has been the design and construction of multi-domain, TN devices, in which regions of right-handed and left-handed twist alternate in the cell. This director structure is imposed by using suitably patterned boundaries [3–9].

While technological advances will likely make their production easier, there are fundamental problems associated with multi-domain TN devices that need to be investigated and understood theoretically. Most notably, because disclinations necessarily appear at the boundary between domains with different handedness, it is natural to expect that the disclination dynamics will play a major role in determining the switching properties of the devices. Understanding the disclination motion is vital in suggesting better device designs.

Therefore in this letter we investigate how disclinations are created, move and are destroyed as two- and four-domain TN devices are switched. To do this we use a lattice Boltzmann algorithm to
solve the three dimensional, Beris-Edwards equations of motion for nematic hydrodynamics. This formalism, where the equations are written in term of a tensor order parameter, allows variation in the magnitude of the order parameter and hence a natural description of the disclination motion. This is a full hydrodynamic treatment which includes the effect of back-flow.

We first consider a two-domain TN device, where stripes of left and right handed twist are separated by disclination lines. We find that the application of an electric field pins the disclination line to one of the two surfaces. The switching on is slightly faster than for a single domain TN. The switching off is, however, considerably slower, as the driving force for the disclination to return to the centre of the device is small. We suggest a novel device geometry aimed at overcoming this problem.

We then present results for a four-domain device, which comprises a checkerboard of TN columns of different handedness. For this geometry a surface pretilt or non-zero voltage are needed to sustain the four-domain director pattern: otherwise the disclinations annihilate leaving, effectively, either a single or two-domain TN device. We find, in agreement with experiments, that for a given initial four-domain state, very small fluctuations determine whether the structure relaxes to a single or two domain TN and we describe the dynamic pathways by which these states are reached. We then follow the way in which disclinations are created, move and interact as the field is switched on. These phenomena occur on the ms time scale.

**Equations of motion.** – The equilibrium properties of the liquid crystal are described by a Landau-de Gennes free energy density \[ f(\mathbf{Q}, \mathbf{E}) = \frac{A_0}{2} (1 - \frac{\gamma}{3})Q_{\alpha\beta}^2 - \frac{A_0\gamma}{3} Q_{\alpha\beta}Q_{\beta\gamma}Q_{\gamma\alpha} + \frac{A_0\gamma}{4} (Q_{\alpha\beta}^2)^2 + \frac{K}{2} (\partial_\alpha Q_{\beta\gamma})^2 + \frac{\epsilon}{2} Q_{\alpha\beta} \mathbf{E}_\alpha \mathbf{E}_\beta \] (1)

where \( K \) is the liquid crystal elastic constant, \( \epsilon > 0 \) for positive dielectric materials (its value fixes the voltage scale, see captions to figures), \( \mathbf{Q} \) is the tensorial order parameter (related to the director field \( \mathbf{n} \) via \( Q_{\alpha\beta} = 3/2(n_\alpha n_\beta - 1/3\delta_{\alpha\beta}) \)) where \( \langle \cdot \rangle \) denote a coarse grained average and \( \delta \) is Kronecker delta [1, 10], \( \mathbf{E} \) is the electric field, \( A_0 \) is a constant and \( \gamma \) controls the magnitude of order (quantified via the largest eigenvalue of \( \mathbf{Q} \)). The equation of motion for \( \mathbf{Q} \) is \( D_t \mathbf{Q} = \Gamma \mathbf{H} \), where \( D_t \) is a suitable material derivative [10], \( \Gamma \) is a collective rotational diffusion constant and \( \mathbf{H} = -\frac{\delta f}{\delta \mathbf{Q}} + (\mathbf{I}/3) Tr \frac{\delta f}{\delta \mathbf{Q}} \). The fluid velocity, \( \mathbf{u} \), obeys the continuity equation and the Navier-Stokes equation with a stress tensor appropriate to liquid crystals (see Ref. [10] for details). The director field configuration may give rise to a non-zero velocity via the stress tensor [10]: this effect is known as backflow. To solve these equations we use a lattice Boltzmann algorithm, the details of which have been given in Refs. [11, 12]. To locate disclination lines, we require that a point in the simulation domain belongs to a disclination if the value of \( q \) there falls below 60% of the average magnitude of order through the sample (the thickness of the disclinations in Figs. 4 and 5 slightly depends on the value of the threshold).

**Two-domain twisted nematic device.** – The boundary patterning necessary to stabilise a TN device is shown in Fig. 1A, together with the definition of the co-ordinate axes we shall use (periodic boundaries are taken along \( x \) and \( y \)). We first consider a two-domain twisted nematic device (2DTN), in which left-handed and right-handed twisted nematic stripes are separated by disclinations. The boundary patterning necessary to stabilise the 2DTN is shown in Fig. 1B. The handedness of different sections of the device is imposed by rubbing the surfaces such that the director field has a \( \pm 2^\circ \) pretilt (ie angle to the \( xy \)-plane).
Fig. 1 – The geometry considered in the text, together with the surface patterning leading to a (a) single domain (b,c) two-domain and (d) four-domain TN device.

Without an electric field, there is a twist disclination line parallel to the $y$ axis at the centre of the cell between domains of opposite handedness. In equilibrium no escape into the third dimension is found at the disclination core in the one elastic constant approximation, if there is no pretilt. If we relax the one elastic constant approximation, e.g. by adding the term $K'(\partial_{z}Q_{\alpha\beta})^2$ to $f$ in Eq. 1 where $K'$ is another elastic constant [1], we find $n_z \neq 0$ at the disclination core ($n_z = 0.08$ for $K'/K = 2$ with other parameters as in Fig. 2).

Our aim is to understand how the disclination affects the switching dynamics. Fig. 2a shows the position of the disclination as a function of time during a cycle of turning the field on, and then off. When the field is switched on the disclination moves quickly to the surface at $z = L$. It is advantageous to accommodate the disclination here because of the particular geometry of the surface pretilt. When the field is switched off, the disclination line moves slowly back to the centre of the device. This is a much slower process because, in zero field the free energy of the state with the disclination at the surface of the device is only slightly higher than that with it at the centre. Therefore the driving force is small and the disclination will be easily pinned en route by any impurities.

We ran simulations with purely relaxational dynamics and compared them to the physical case where movements of the director can induce flow fields in the device. The results are compared in Fig. 2. The effect of backflow is to delay the onset of switching when the field is applied but to enhance the speed of the disclination once it starts to move. Backflow also increases the speed with which the disclination returns to the centre of the device when the field is switched off.

While the switching on is slightly faster for the two-domain device than for a conventional single-domain TN device with the same conditions, the switching off is substantially slower as the disclination takes a long time to move back to the centre of the cell. This is obviously deleterious to its operation as a fast display. To overcome this problem we propose a two-domain device where the domain structure is stabilised by a surface $\pi/2$ pre-twist (see Fig. 1c). The disclinations now remain at the surface in both the on and off states.

Fig. 3 compares switching in two-domain devices with pre-tilt (as in Fig. 1b) and with a $\pi/2$ surface pre-twist (as in Fig. 1c), with identical parameters. The value of the director in the $xy$ plane and along the $z$-axis are shown as a function of time. Both devices would lead to a comparable viewing angle improvement over the single domain cell. The pre-twist device switches on as quickly as the pre-tilt device. However it avoids the slow switching off of the pre-tilt device.

**Four-domain twisted nematic device.** – We now consider how disclination dynamics influences the switching of a four-domain TN (4DTN) liquid crystal device. In such a device the target is to obtain a configuration in which columns of left- and right-handed twist are organised in a checkerboard pattern. The rubbing directions we consider are shown in Fig. 1d: this mimicks the
Fig. 2 – Switching dynamics in a 2DTN device. The plot shows the time evolution of the $z$ position of the disclination, for the two cases with and without backflow. Parameters are $K = 25 \text{ pN}$, $L = 1.5 \text{ \textmu m}$, $\gamma = 3$, the average magnitude of order is $q = 0.5$, the applied voltage is $2.4 \text{ } V_c$, where $V_c$ is the Freedericksz threshold [1] (in a Freedericksz cell with the same parameters), and there is a pretilt of $2^\circ$ at the surfaces. We used $A_0/(KL^2) = 7 \times 10^{-4}$. The rotational and isotropic viscosities (see Ref. [12]) are $\gamma_1 = 1$ and $\eta = 0.03 \text{ Poise}$. The field was switched on at $t = 0$ and off at $t = 2.7 \text{ ms}$. The inset shows the switching on dynamics.

Fig. 3 – Comparison between switching dynamics in a two-domain twisted nematic device as in Fig. 1b, and in another one as in Fig. 1c, in which the disclination is at the surface for all times. The plot shows the time evolution of the $z$ component of the director field along $z$ ($n_z$, left) and of its larger component on the $xy$ plane ($n_x$, right). Backflow is not considered. Here $L = 0.75 \text{ \textmu m}$, $V = 1.92 \text{ } V_c$. Other parameters are as in Fig. 2.
Fig. 4 – Two annihilation pathways in a 4DTN device with a pretilt \( t_0 = 10^\circ \) for \( V < V_{\text{min}}(t_0) \) so that the disclinations annihilate. Only the midplane of the device \( (z = L/2) \) is shown as the disclinations are confined there throughout the simulation. These pathways correspond to those experimentally observed in Ref. [5]. Parameters are: \( K = 25 \) pN, \( L = 1 \) \( \mu \)m, \( \gamma = 3 \) and \( \gamma_1 = 1 \) Poise. The average magnitude of order is 0.5. We used \( A_0/(KL^2) = 0.025 \). Applied voltages are: 0.75 \( V_c \) (top) and 0.15 \( V_c \) (bottom), \( V_c \) being the Freedericksz threshold (as in Fig. 2). The domain dimension is \( 2d \times 2d = 3.2 \) \( \mu \)m \( \times 3.2 \) \( \mu \)m.

experential set-up chosen in Refs. [4]. Note that, unlike the 2DTN device, the two surfaces of the 4DTN device can carry the same patterning. A related theoretical study, within the Ericksen-Leslie theory, has been proposed in Ref. [9].

In the 4DTN device, the pre-tilt angles on or near the surfaces are crucial to the stabilization of the director field configuration. This can be understood within a simple model [4]. Creating the disclinations increases the free energy and therefore the surface must be rubbed with a non-zero pretilt, \( t \), so that removing the disclinations will lead to a greater free energy penalty: if there is no pretilt the 4DTN display is never stable but unwinds. There is a finite critical threshold for the pretilt, \( t_{\text{min}} \), which can stabilise the structure at zero voltage. This depends on the geometry of the device [4]. For a pretilt \( t \) smaller than \( t_{\text{min}} \), the four-domain structure is not stable at low voltages. Experiments [4] and theory [4, 9] show however that, even for \( t < t_{\text{min}} \), the 4DTN device is stable for voltages above a certain threshold \( V_{\text{min}}(t) \).

In our numerical simulations, we consider a pretilt \( t_0 = 10^\circ \) which is less than \( t_{\text{min}} \). For voltages smaller than \( V_{\text{min}}(t_0) \sim 0.9 \) \( V_c \) (\( V_c \) is the Freedericksz threshold) the four domain structure is not stable and reduces to what is effectively a single domain or a two-domain twisted configuration. The single domain has lower free energy, but the two domain structure is also a local minimum. Typical pathways followed by the disclination lines as the 4DTN structure unwinds, are shown in Fig. 4. It is to be stressed that the different pathways follow from identical initial conditions: which pathway is followed depends solely on (numerical) noise. These patterns resemble those observed in the experiments in [4].
Fig. 5 – Evolution of the disclination configuration as a 4DTN device is switched on from the stable disclination free configuration (frames 1a-1d) and from the metastable configuration shown in Fig. 4 (second row) (frames 2a-2d). The voltage at $t = 0$ is smaller than $V_{\text{min}}(t_0)$. It is changed to a value larger than $V_{\text{min}}(t_0)$ after 6.7 or 13.4 ms for the pathways 1 and 2 respectively. The voltages are 0.60 $V_c$ and 1.79 $V_c$ for frames (1a-1d) and 0.15 $V_c$ and 1.34 $V_c$ for frames (2a-2d). The time, measured from the moment the voltage has been increased, is shown above each frame. The domain dimension is 1.6 $\mu$m × 1.6 $\mu$m for the first pathway and 3.2 $\mu$m × 3.2 $\mu$m for the second. $L = 0.5$ (and $A_0/(KL^2) = 0.025$) and 1 $\mu$m (and $A_0/(KL^2) = 0.1$) for the top and bottom pathways, while other parameters are as in Fig. 4.

Above $V_{\text{min}}(t_0)$, the 4DTN device is stable and there are well-defined columns of right and left-handed twist. Our simulations show however that at these voltages the disclinations no longer lie at the centre of the cell but pin to the top or bottom surfaces between the regions of different pretilt in such a way that they do not cross. Near the centre of the cell there is a large component of the director field along the $z$ direction.

We now describe the dynamics of the switching from the off state in which the voltage is below the critical value (and $t < t_{\text{min}}$ so the four-domain structure has collapsed), to the on state in which the disclinations are pinned at the device boundaries. In Fig. 5 we show the dynamical switching pathways starting from a stable disclination-free configuration (frames 1a-1d), and from the metastable configuration shown in Fig. 4 (frames 2a-2d).
In the first case, disclination loops are created in the middle of the sample. These loops then grow (Fig. 5, frame (1b)) until they touch the boundaries and then approach each other sufficiently closely that they can interact (frame 1c). They annihilate at the centre of the device and merge at the boundaries to form the pinned disclination pattern characterising the large voltage stable state. A similar switching mechanism was postulated in [9].

In the second case shown in Fig. 5, frames 2a-2d, two disclinations are present at the beginning of the simulation in a metastable starting state. This configuration is likely to be present in the experiments in some regions of the sample [4]. After the voltage is increased above the critical threshold, the disclinations bend (frame 2a) and different sections of the disclination lines start moving to the two surfaces. During this motion, the disclinations acquire a non-zero twist (frames 2b-2c). The disclinations distort when they touch the boundary and move towards the stable configuration, which is again reached by merging the disclinations at the boundaries and annihilating those at the centre of the cell.

Discussions and conclusions. – In conclusion, we have solved numerically the hydrodynamic equations of motion to show that in the two- and four- domain TN devices disclination dynamics is crucial to the switching. We hope that understanding the disclination motion will prove useful in improving the design of multi-domain TN devices. For example, in the two-dimensional TN device, we found that the switching off is slowed considerably by having to wait for the disclination to return to the centre of the cell. We showed that, if the surfaces are patterned with an alternating large “pre-twist” (in a manner similar to that described for related multi-domain devices in [7]), the disclinations sit at the surface of the device even at zero voltage. Hence switching occurs without any need to rearrange the disclination pattern, thus circumventing the long time needed for switching off whilst preserving the viewing angle advantages of the two-domain device. This and the other predictions made here could be tested in devices of suitable dimensions, by deducing the disclination line position from the time dependent optical properties of the sample.

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