DYNAMICAL FLOW EFFECT IN TWISTED NEMATIC LIQUID CRYSTAL CELLS

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Abstract—We numerically solve the Ericksen-Leslie hydrodynamic equations for a number of twisted nematic liquid crystal cells. We show that when an applied electric potential is varied abruptly across the cell, the resulting fluid motion can play a critical role in inducing the rotation of directors. The physics underlying the seemingly abnormal behavior of director rotation is investigated.

I. INTRODUCTION

The significance of flow effect in twisted nematic liquid crystals (LC) was first demonstrated by van Doorn and Berreman in a theoretical explanation of the "bounce" phenomenon observed in the light transmission of a LC cell sandwiched between cross polarizers [1,2]. The experimental observation is that when an applied voltage is switched off in a cell with a $\pi/2$ -twist, the directors in the central part of the cell can tilt past the substrate normal, opposite to the relaxation direction, and the director configuration experiences a transition from an initial $\pi/2$ -twist to a momentary $-3\pi/2$ -twist, opposite to that of the equilibrium state without an applied voltage. Here Φ -twist means that for a given configuration of $\mathbf{n} \equiv (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, the twist angle, defined as $\int_0^d d\phi(z)$, equals to Φ , with z-axis being the substrate normal and d the cell thickness. The starting point of the numerical computation is the hydrodynamic equations of Ericksen and Leslie. A comparison between the results obtained with and without the fluid motion shows that under certain circumstances, dynamical flow can play a critical role in governing the rotation of the directors. However, though the numerical results in Ref. [1,2] have undoubtedly demonstrated the observed effect, a physical picture is still lacking.

The purpose of this paper is to obtain a physical picture of dynamical flow pattern and its effect on director rotation. We have re-examined the case studied in Ref. [1,2] and demonstrated that similar flow effect can occur in other types of twisted LC cells. We find they all have the same basic physical mechanism, consisting of two components. The first component is that right after the applied potential is switched off, the flow velocity field near the two substrates is induced by the fast rotation of the directors. This is because the gradient of director orientation is largest at these places. Due to angular momentum conservation, the flow field must obey certain symmetry relations about the mid-plane, in order for the overall angular momentum to be zero. In particular, it means the velocity gradient at mid-plane is opposite to that close to the substrates. The coupling of the director to the gradient of the flow field (via the viscous molecular field) thereby implies that the rotation of the directors throughout the central part of the cell is "anomalous."

II. MECHANISM OF DYNAMICAL FLOW EFFECT

A. Hydrodynamical equations

The hydrodynamic equations of Ericksen and Leslie are

$$\partial_t(\rho v_i) + \partial_j(\rho v_i v_j + p \delta_{ji} - \sigma_{ji}^d - \sigma_{ji}^f - \sigma_{ji}') = 0, \quad (1)$$

$$Id^2 n_i / dt^2 = h_i + h_i' + \gamma n_i, \quad (2)$$

where σ^d is the stress tensor from elastic distortion, σ^f the stress tensor induced by electric and magnetic fields, σ' the viscous stress tensor, and $\mathbf{h}$ is the molecular field from elastic distortion and (order parameter) field free energy, $\mathbf{h}'$ the viscous molecular field and γ is a Lagrangian multiplier. Omitting the inertial terms [1,2], we have

$$\begin{aligned} \partial_3 \sigma'_{31} &= 0, \\ \partial_3 \sigma'_{32} &= 0, \end{aligned} \quad (3)$$

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$$\mathbf{n} \times (\mathbf{h} + \mathbf{h}') = 0 \quad (4)$$

where the substrate normal is defined as z-axis and the space-dependence of all the quantities is on z only. Here the fluid motion is in-plane motion, hence the velocity components $v_1 \neq 0$ and $v_2 \neq 0$ only. Note that $\sigma_{31}^d = \sigma_{32}^d = 0$ as only $\partial_3 \mathbf{n} \neq 0$ and $\sigma_{31}^f = \sigma_{32}^f = 0$ as the applied fields are along z-axis. Explicit expressions for the quantities in Eqs. (1) and (2) can be found in Ref. [3]. The boundary conditions are that at the substrates, the velocity components vanish and the directors are given constants. The material parameters used in the present numerical computation are taken from Ref. [1], suitable for MBBA doped with 2% dimethylaminobenzonitrile.

B. Dynamical symmetry

We have numerically solved the hydrodynamic equations for the two types of cells with twist angles $\pi/2$ and π , which are dictated by the boundary conditions for the directors at the lower and upper substrates. The following dynamical symmetries were found and proved to be rigorous analytically. With the directors at the lower and upper substrates denoted by $\mathbf{n}_L$ and $\mathbf{n}_U$, as $n_{L1} = n_{U2}$ and $n_{L2} = n_{U1}$ (for the cell with twist angle $\pi/2$, $n_{L1} \simeq 1$ and $n_{U2} \simeq 1$), then the time-varying directors and velocities will obey the relations

$$\begin{aligned} n_1(z) &= n_2(d-z), \\ n_2(z) &= n_1(d-z), \\ n_3(z) &= n_3(d-z), \\ v_1(z) &= -v_2(d-z), \end{aligned} \quad (5)$$

provided the initial state has such symmetries. If $n_{L1} = -n_{U1}$ and $n_{L2} = n_{U2}$ (for the cell with twist angle π , $n_{L1} \simeq 1$ and $n_{U1} \simeq -1$), then the time-varying directors and velocities will obey the relations

$$\begin{aligned} n_1(z) &= -n_1(d-z), \\ n_2(z) &= n_2(d-z), \\ n_3(z) &= n_3(d-z), \\ v_1(z) &= v_1(d-z), \\ v_2(z) &= -v_2(d-z), \end{aligned} \quad (6)$$

provided the initial state possesses the above symmetries.

C. Dynamical flow effect on director rotation

When a strong electric potential is applied across the cell, the field coherence length $\sqrt{4\pi K_{11}/\epsilon_a E^2}$ can be much smaller than the cell thickness d . Here ϵ_a is the dielectric anisotropy and E is the field strength. As a consequence, the directors near the substrates can exhibit large elastic distortions, leaving the directors throughout the central part of the cell (nearly) uniformly vertical. When the voltage is switched off, the local elastic distortion energy density near the

substrates can be much higher than its value at the equilibrium state. The instantaneous (elastic distortion) molecular field $\mathbf{h}$ is therefore very large near the substrates and can thus give rise to the fast rotation of the directors. This fact is confirmed by the time-varying configuration of the directors. The near-substrate rotation of the directors will inevitably induce a flow velocity field due to the coupling between $\mathbf{n}$ and $\mathbf{v}$ through the viscosity relations. In the law of friction, the forces are proportional to the fluxes, one of which is just the conventional $\partial_i v_j + \partial_j v_i$ and the other is $\mathbf{N} = \dot{\mathbf{n}} - \boldsymbol{\omega} \times \mathbf{n}$ with $\boldsymbol{\omega} = \nabla \times \mathbf{v}/2$. It is the latter which determines the rotational field $\boldsymbol{\omega}$ near the substrates. In all the cases we have studied, it is found that the near-substrate $\dot{\mathbf{n}}$ always locally induces a $\boldsymbol{\omega} \times \mathbf{n}$ in the same direction, which means $\boldsymbol{\omega}$ is parallel to $\mathbf{n} \times \dot{\mathbf{n}}$. The knowledge of the near-substrate $\boldsymbol{\omega} = (-\partial_3 v_2, \partial_3 v_1, 0)$, plus the boundary conditions and the dynamical symmetry relations, are sufficient to qualitatively determine the whole velocity field in the cell. The spatial variation of the velocity field near the middle plane is therefore completely deduced. This is illustrated in Fig. 1 for the π -twist cell, in which $\theta = 92^\circ$, $\phi = 2^\circ$ and $\theta = 92^\circ$, $\phi = 178^\circ$ at the lower and the upper substrates respectively. Right after the potential is switched off, $\dot{\mathbf{n}}$ near the substrates is expected to be along the negative z direction. The near-substrate $\boldsymbol{\omega}$, in the direction of $\mathbf{n} \times \dot{\mathbf{n}}$, will have $\partial_3 v_1 > 0$, $\partial_3 v_2 > 0$ near $z = 0$ (the lower substrate), and $\partial_3 v_1 < 0$, $\partial_3 v_2 > 0$ near $z = d$ (the upper substrate). With the help of the dynamical symmetry relations, we can deduce the qualitative variations of v_1 and v_2 as depicted in Fig. 1. The effect of angular momentum conservation is clearly present. Thus the source of dynamical symmetry relation may be understood as arising from a conservation law. As the directors throughout the central part of the cell are nearly homogeneous and hence the molecular field due to elastic distortion is weak (even in the presence of natural helicity), their motion can only be driven by the gradient of the flow field, which is opposite to that close to the substrates. It is quantitatively confirmed that just after the electric field is switched off, the magnitude of the viscous molecular field $\mathbf{h}'$ at mid-plane is more than ten times larger than that of elastic molecular field $\mathbf{h}$.

For the cell with $\pi/2$ -twist, the results in Ref. [1] can be used to verify the mechanism described above. For the cell with π -twist, the numerical results are depicted in Figs. 1 and 2. Essentially, again after a strong electric voltage is switched off, the directors near the middle plane tilt past the substrate normal and the whole $\mathbf{n}$ configuration experiences a transition from π -twist to $-\pi$ -twist, which is in the opposite sense to that of the equilibrium state in the absence of the electric field. The common feature of the above two cases is that the dynamical flow is induced as the electric voltage is switched off and this flow can drive the director configuration into a mo-

Fig. 1. Space and time dependences of flow velocity components v_1 and v_2 after potential 17.5 V is turned off. Velocity is in unit of $K_{11}/d\alpha_4$ and space coordinate in unit of d . Time interval between adjacent curves is 0.005 sec. Note that velocity amplitude decreases monotonically with time everywhere.

Fig. 2. Time-evolution of the n_2 component at mid-plane after a potential of 17.5 V is switched off. Note that $n_1 = 0$ at any time due to the dynamical symmetry.

mentary twist which differs by 2π from that of the equilibrium state the system finally reaches. Here we want to point out that though the results depicted in Ref. [1] and this paper are only for LC without natural helicity, the mechanism proposed here has also been verified for LC of various natural pitches with the boundary conditions specified above. It is worth noting that as its manifestation, dynamical flow effect studied here does not inevitably lead to momentary twist which is different from the original one or the one at equilibrium.

III. DISCUSSION

Nematic structures, which have 2π difference in twist angle, can exhibit distinguishable optical responses. Since momentary twist different from the original one can be reached with the help of dynamic

flow induced by abrupt voltage switching off, it is therefore of interest to investigate if certain substrate and helicity conditions can keep the momentary twist in further relaxation and so lead to an equilibrium state with twist angle different from the initial state in the absence of electric field. On this basis, a switching bistability may be realized.

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