Electronic Supplementary Material (ESI) for Soft Matter.

Electrically controlled topological micro cargo transportation

Supplementary Information File F2

Theoretical Model

I. INTRODUCTION

We consider a Hybrid Aligned Nematic (HAN) cell with zero pretilt so that the two HAN states are energetically equivalent. In the absence of any other forcing either state will form, with defects in between each domain.

With an interdigitated electrode (IDE) structure on the substrate we have the ability to create an electric field structure that produces a preference for particular HAN states at particular locations within the cell. Specifically, at the two edges of an electrode the field direction means that different HAN states are preferred. It is then possible for a defect to be formed in the inter-electrode gap. A sketch of the different HAN states is shown in Fig. 1(a) and a more accurate simulation of the director structure, including the location of the defects (darker green areas above the middle of the electrode at $y = 0$ and above the gap at $y = \lambda/2$) is included in Fig. 1(b). We will consider a model where the electric field affects

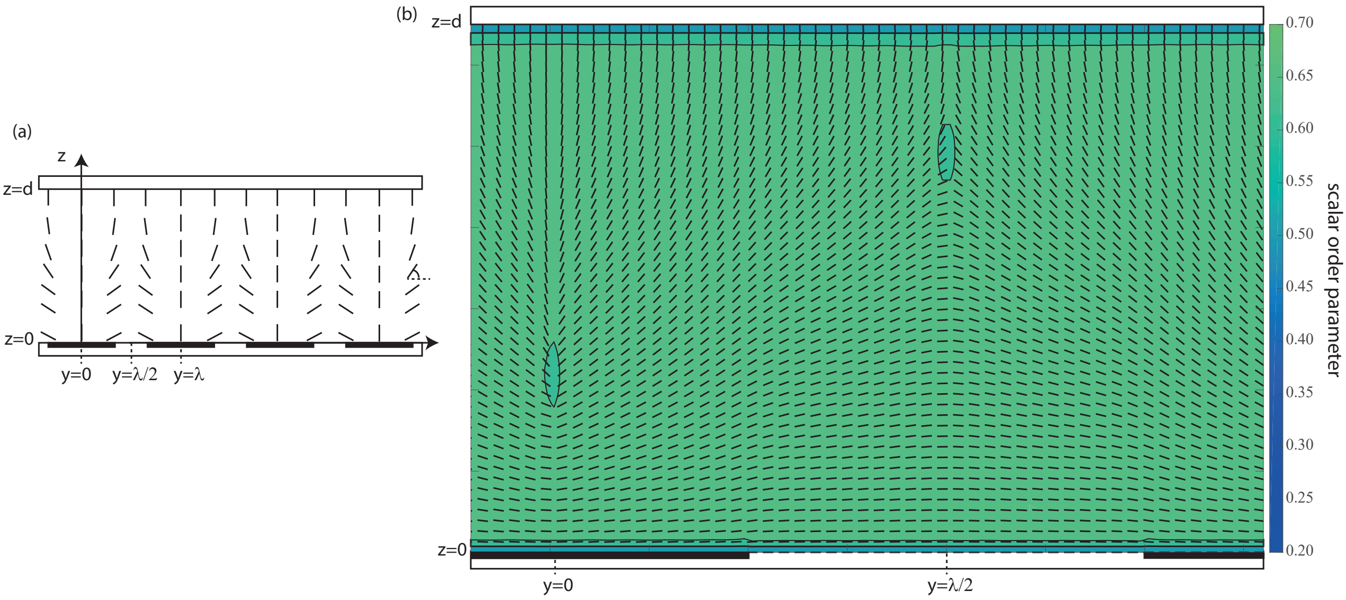

FIG. 1: (a) Sketch of the preferred director structure induced by the electric field obtained from an interdigitated electrode structure of wavelength λ, in a cell of thickness d. The x-extent of the cell is taken to be $0 \leq x \leq L$. (b) $\mathbf{Q}$-tensor calculation of the 2-dimensional director configuration. The regions of low order, (darker green areas above the middle of the electrode at $y = 0$ and above the gap at $y = \lambda/2$) indicate the presence of $+1/2$ defects.

the director close to the IDE substrate but, due to the decay in field strength away from the IDE, has little effect on the director in the bulk of the cell. With this approximation the bulk director structure is influenced only by elastic effects with the director close to the substrate being also influenced by anchoring and field effects. We assume a director of the form $\mathbf{n} = (0, \cos(\theta), \sin(\theta))$ so that if the director was a HAN-like state uniformly in the xy-plane then the director angle would be

$$\theta(z) = \left(\theta_0 + \left(\frac{\pi}{2} - \theta_0\right)\frac{z}{d}\right), \tag{1}$$

where θ_0 is the director angle at the lower substrate. If we now assume that elastic effects in the xy-plane are smaller than in the z-direction, because of the shallow aspect ration of the cell ($d/\lambda \ll 1$), then we can say that the director structure is parameterised by the substrate director angle θ_0, which we now assume varies in the xy-plane due to the IDE field structure. We therefore consider a dynamic director structure,

$$\theta(x, y, z, t) = \left(\theta_0(x, y, t) + \left(\frac{\pi}{2} - \theta_0(x, y, t)\right)\frac{z}{d}\right). \tag{2}$$

We now consider each energy contribution in detail. By prescribing the form of the z-dependance of the director angle θ, and then averaging over the z-direction, we are able to develop a 2-dimensional model which governs the variation of the director angle at the lower substrate, $\theta_0(x, y, t)$, in the xy-plane.

II. ENERGY

A. Elastic Energy

In a one constant approximation the Frank elastic energy will be

$$E_{\mathrm{f}} = \int_0^L \int_0^{2\pi n/\lambda} \int_0^d \frac{K}{2}\left(\left(\frac{\partial\theta}{\partial x}\right)^2 + \left(\frac{\partial\theta}{\partial y}\right)^2 + \left(\frac{\partial\theta}{\partial z}\right)^2\right) dx\, dy\, dz, \tag{3}$$

where K is the average Frank elastic constant. If we now assume a director structure as given in eq. (2) this energy becomes

$$E_{\mathrm{f}} = \int_0^L \int_0^{2\pi n/\lambda} \frac{K}{2}\left(\frac{d}{3}\left(\left(\frac{\partial\theta_0}{\partial x}\right)^2 + \left(\frac{\partial\theta_0}{\partial y}\right)^2\right) + \frac{1}{d}\left(\frac{\pi}{2} - \theta_0\right)^2\right) dx\, dy. \tag{4}$$

B. Anchoring energy

The form of the director structure in eq. (2) assumes that the director at the upper homeotropic substrate is rigidly anchored, or that the elastic and electric field effects there are weak and director distortion is negligible. We do not, therefore, need to specify a surface anchoring energy at the upper surface. However, the electric field effects at the lower substrate are stronger and we assume weak planar anchoring at the lower substrate. The appropriate energy is therefore,

$$E_{\mathrm{a}} = \int_0^L \int_0^{2\pi n/\lambda} \frac{W_0}{2} \left(\sin^2\left(\theta(x, y, 0, t)\right)\right) dx\, dy, \tag{5}$$

where W_0 is the anchoring strength at the lower substrate. With our approximate director angle, eq. (2), this becomes,

$$E_{\mathrm{a}} = \int_0^L \int_0^{2\pi n/\lambda} \frac{W_0}{2} \left(\sin^2\left(\theta_0\right)\right) dx\, dy. \tag{6}$$

C. Electrostatic energy

We assume that the electric field is of the form

$$\mathbf{E} = E(y, z)(0, \cos(\phi(y)), \sin(\phi(y))), \tag{7}$$

so that the field direction, ϕ, is only a function of y due to the electrode structure, and that the field strength, E, is a function of y and z, i.e. it decays into the cell (z-dependence) and is periodic in y due to the IDE. The electrostatic energy can then be approximated as,

$$E_{\mathrm{e}} = -\int_0^L \int_0^{2\pi n/\lambda} \int_0^d \frac{\epsilon_0 \Delta\epsilon}{2} (\mathbf{E}\cdot\mathbf{n})^2 dx\, dy\, dz \tag{8}$$

$$= -\int_0^L \int_0^{2\pi n/\lambda} \int_0^d \frac{\epsilon_0 \Delta\epsilon}{2} E(y, z)^2 \cos^2(\theta(x, y, z, t) - \phi) dx\, dy\, dz. \tag{9}$$

Even with a simplified form of the director this is a non-integrable function of z. We therefore approximate the electric field effect by averaging in the z direction, modelling the effect purely through the interaction between the electric field angle ϕ and the director in the middle of the cell θ_m. The electric energy then reduces to

$$E_{\mathrm{e}} = -\int_0^L \int_0^{2\pi n/\lambda} \frac{\epsilon_0 \Delta\epsilon d}{2} E(y)^2 \cos^2(\theta_m - \phi) dx\, dy. \tag{10}$$

From Fig. 1 we can approximate the periodic field direction as $\phi = \dfrac{\pi}{2} - \dfrac{\pi}{\lambda} y$ and so the energy becomes,

$$E_{\mathrm{e}} = -\int_0^L \int_0^{2\pi n/\lambda} \frac{\epsilon_0 \Delta\epsilon d}{2} E(y)^2 \sin^2\left(\theta_m + \frac{\pi}{\lambda} y\right) dx\, dy. \tag{11}$$

D. Total energy

The total energy is therefore,

$$
\begin{aligned}
E &= E_{\mathrm{f}} + E_{\mathrm{a}} + E_{\mathrm{e}} \\
&= \int_0^L \int_0^{2\pi n/\lambda} \frac{K}{2}\left(\frac{d}{3}\left(\left(\frac{\partial \theta_0}{\partial x}\right)^2 + \left(\frac{\partial \theta_0}{\partial y}\right)^2\right) + \frac{1}{d}\left(\frac{\pi}{2} - \theta_0\right)^2\right) \\
&\qquad + \frac{W_0}{2}\left(\sin^2(\theta_0)\right) - \frac{\epsilon_0 \Delta\epsilon d}{2} E(y)^2 \sin^2\left(\theta_m + \frac{\pi}{\lambda} y\right) dx\, dy. \qquad (12)
\end{aligned}
$$

III. DISSIPATION

The rate of dissipation in the cell, assumed to be purely due to director rotation rather than viscous effects, is

$$
D = \int_0^L \int_0^{2\pi n/\lambda} \int_0^d \gamma_1 \left(\frac{\partial \theta}{\partial t}\right)^2 dx\, dy\, dz, \qquad (13)
$$

which, with our approximate director structure, eq. (2), becomes,

$$
D = \int_0^L \int_0^{2\pi n/\lambda} \frac{\gamma_1 d}{3} \left(\frac{\partial \theta_0}{\partial t}\right)^2 dx\, dy. \qquad (14)
$$

IV. GOVERNING EQUATION

Using a Rayleigh dissipation principle the governing equation for $\theta_0(x, y, t)$ then becomes

$$
\frac{\gamma_1 d}{3}\frac{\partial \theta_0}{\partial t} = K\left(\frac{d}{3}\left(\frac{\partial^2 \theta_0}{\partial x^2} + \frac{\partial^2 \theta_0}{\partial y^2}\right) + \frac{1}{d}\left(\frac{\pi}{2} - \theta_0\right)\right) - \frac{W_0}{2}\sin(2\theta_0) + \frac{\epsilon_0 \Delta\epsilon d}{2} E(y)^2 \sin\left(2\left(\theta_m + \frac{\pi}{\lambda} y\right)\right) \qquad (15)
$$

Note that if the director structure in eq. (2) is parameterised by θ_m, the mid-cell director angle, then, since

$$
\theta_m = \left(\frac{\pi}{4} + \frac{\theta_0(x, y, t)}{2}\right), \qquad (16)
$$

this governing equation, using the short hand $u = \theta_m$ so that $\theta_0 = 2u - \pi/2$, becomes

$$
\frac{2\gamma_1 d}{3}\frac{\partial u}{\partial t} = K\left(\frac{2d}{3}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + \frac{(\pi - 2u)}{d}\right) + \frac{W_0}{2}\sin(4u) - \frac{\epsilon_0 \Delta\epsilon d}{2} E(y)^2 \sin\left(2\left(u + \frac{\pi}{\lambda} y\right)\right) \qquad (17)
$$

The final elastic term, $K(\pi - 2u)/d$, is an elastic effect which attempts to create a uniform director structure in the z-direction, which, because $\theta = \pi/2$ at the top boundary, means that the state $\theta_0 = \pi/2$ (or $u = \pi/2$) is elastically preferred. If we non-dimensionalise using $x = dX$, $y = dY$, $t = (d^2\gamma_1/K)T$, then

$$\frac{\partial u}{\partial T} = \frac{\partial^2 u}{\partial X^2} + \frac{\partial^2 u}{\partial Y^2} + \frac{3}{2}(\pi - 2u) + \frac{3W_0 d}{4K}\sin(4u) - \frac{3d^2\epsilon_0\Delta\epsilon}{4K}E(Y)^2\sin\left(2\left(u + \frac{\pi d}{\lambda}Y\right)\right). \tag{18}$$

The form of the electric field $E(Y)$ could be approximated as a constant, and related to V/λ but may more accurately be prescribed from Comsol simulations of the electric field in an isotropic dielectric IDE cell to take account of fringing fields (Fig. 2). From these simulations

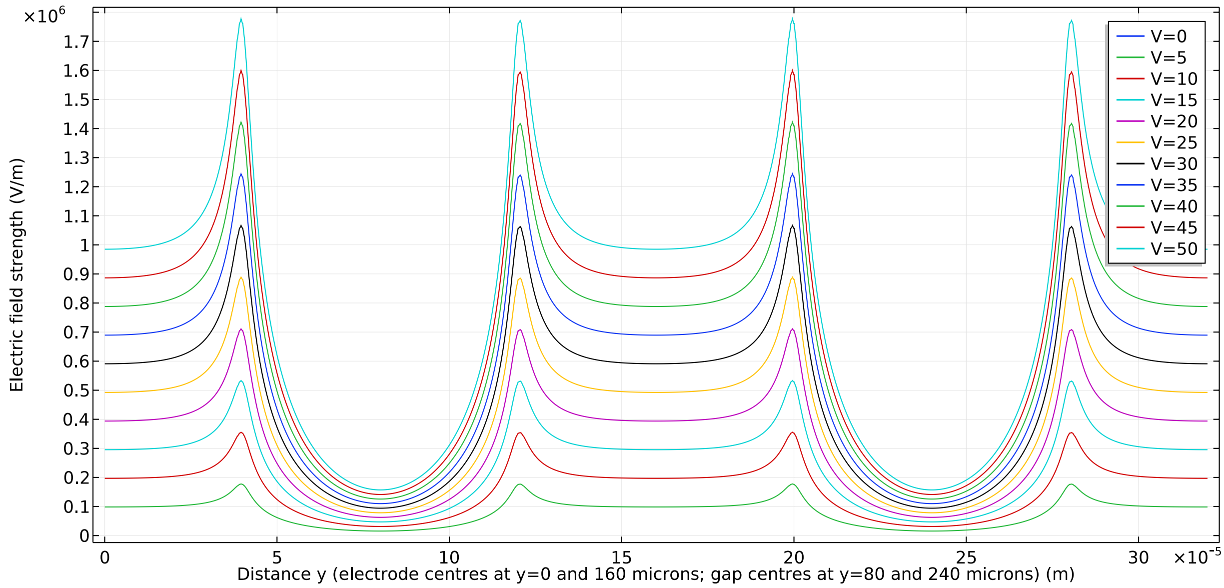

FIG. 2: Plot of electric field strength at $z = 1.3 \times 10^{-6}m$ into a $d = 13 \times^{-6} m$ isotropic dielectric cell with IDE electrodes (80 micron electrodes, 80 micron gaps) for Voltage 0-50V.

we see that an extremely good approximation is obtained through a linear dependence on voltage so that $E(y) \approx V\,F(Yd/\lambda)$, and where $F(Yd/\lambda)$ is obtained numerically.

Dynamic, two-dimensional solutions for the director angle at the substrate $\theta_0(x, y, t)$, or equivalently for the mid-layer director angle $\theta_m = u(X, Y, t)$, are therefore obtained through the solution of the dimensional eq. (15) or the non-dimensional eq. (18) respectively, with a numerical approximation for $E(y) \approx V\,F(Yd/\lambda)$.