Liquid Crystal Pretilt Control by Inhomogeneous Surfaces

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Abstract

We consider the pretilt alignment of nematic liquid crystal (LC) on inhomogeneous surface patterns comprising patches of homeotropic or homogeneous alignment domains, with azimuthal anisotropy assumed in the surface plane. We found that the resultant LC pretilt generally increases continuously from the homogeneous limit to the homeotropic limit as the area fraction of the homeotropic region increases from 0 to 1. The variations are qualitatively different depending on how the distance between patches compares to the extrapolation length of the stronger anchoring domain. Our results agree with those previously found in stripped patterns. The present findings may provide useful guidelines for designing inhomogeneous alignment surfaces for variable LC pretilt control - a subject of much technological interest in recent years.

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Study of inhomogeneous surfaces for liquid crystal (LC) alignment has witnessed a rapid growth in recently years. Experiments showed that these surfaces could have unique applications as in the making of multi-stable display devices and the control of LC pretilt alignment. This type of alignment surfaces generally comprise two kinds of domains favoring different LC orientations. Majority of theoretical treatments had dealt with domains arranged in alternating stripped or checkerboard patterns. No systematic calculation has been carried for a patchy pattern, which is more likely achieved by non-lithographic techniques that are less costly. In this letter, we perform an extensive simulation study on the alignment of nematic LC on surfaces containing patches of homogeneous or homeotropic alignment domains, with one embedded in the matrix of the other.

Figure 1 shows the inhomogeneous alignment surfaces we studied for different area fractions of the homeotropic region, $p$. We consider a cubic simulation cell with sides of unity filled with nematic LC. The lower ($z = 0$) surface is the patterned surface as shown in Fig. 1 and the upper surface is free. The cell is assumed to repeat in the $x$ and $y$ directions. If each type of domain has surface energy $W_i(\theta, \phi) (i = 1, 2)$, the unit-area surface energy, $F_s$, would be:

$$F_s(\theta(r), \phi(r)) = \delta(z) \sum_{i=1}^{2} f_i(x, y)W_i(\theta(r), \phi(r)).$$

(1)

Here, $r = (x, y, z)$ is a position vector in the simulation cell; the LC director field is denoted by $\mathbf{n}(r) \equiv (\cos \theta \cos \phi, \cos \theta \sin \phi, \sin \theta)$, where $\theta(r)$ and $\phi(r)$ are, respectively, the zenithal (measured from the surface instead of the surface normal) and azimuthal angles of the LC director; $f_i(x, y)$ is one if $(x, y)$ belongs to domain $i$ and zero otherwise so that the area fraction of domain $i$ is obtainable by integrating $f_i(x, y)$ over the $z = 0$ unit surface. Since our focus is in the LC zenithal (pretilt) alignment produced by the inhomogeneous surface, we impose anisotropy in the $x$-$y$ plane, i.e., both domains prefer the same azimuthal orientation along, say, $\phi_0$. We further assume the local preferred zenithal alignment of domain 1, $\theta_{01} = 88^\circ$ and that of domain 2, $\theta_{02} = 6^\circ$ to lift the foreseen degeneracy between the $\phi(r) = \phi_0$ and $\phi(r) = \phi_0 + 180^\circ$ states. With these assumptions, the azimuthal orientation of the LC is constant in space and equal to $\phi_0$. Hence the surface energy depends only on $\theta(r)$. We use the Rapini-Papoular form of the LC surface energy, $W_i(\theta, \phi_0) = \frac{1}{2}W_{\theta i}\sin^2(\theta - \theta_{0i})$ where $W_{\theta i}$ is the polar anchoring strength of domain $i$. For the LC elastic energy density,
For, we assume the the Frank-Oseen form:

\[ F_e(n) = \frac{1}{2}\{K_{11}(\nabla \cdot n)^2 + K_{22}(n \cdot \nabla \times n)^2 + K_{33}(n \times \nabla \times n)^2\}. \tag{2} \]

Here \( K_{11} \), \( K_{22} \) and \( K_{33} \) are the splay, twist and bend elastic constants, respectively, for which the values of the nematic 5CB are used in simulations \[8\]: \( K_{11} = 7.0 \times 10^{-12} \text{N}, \ K_{22} = 3.5 \times 10^{-12} \text{N}, \ K_{33} = 1.0 \times 10^{-11} \text{N}. \) If the size of the cubic cell were scaled to \( \lambda^3 \), the total energy per unit area is given by

\[ \frac{F_{\text{tot}}(n)}{\lambda^2} = \frac{K_{11}}{\lambda} \left\{ \int_0^1 \int_0^1 \int_0^1 \tilde{F}_e(n) dxdydz + \sum_{i=1}^2 \int_0^1 \int_0^1 \frac{\lambda}{\ell_{ei}} f_i(x, y) \sin^2(\theta - \theta_{0i}) dxdy \right\}, \tag{3} \]

where \( \tilde{F}_e \equiv F_e/K_{11}, \ \ell_{ei} \equiv K_{11}/W_{\theta i} \) is the extrapolation length of the domain \( i \). Equation (3) shows that for the same LC material, the energy density of the system generally increases with \( (1/\lambda) \), but the critical parameter determining the LC configuration is the ratio \( \lambda/\ell_e \) (where \( \ell_e \) is the smaller of \( \ell_{ei} \)): If \( \lambda/\ell_e \ll 1 \), the elastic energy would dominate the surface energy, and vice versa in the opposite limit. For typical alignment surfaces, the polar anchoring energy is \( 10^{-4} - 10^{-3} \text{Jm}^{-2} \) and hence \( \ell_e \approx 0.01 - 0.1 \mu\text{m} \). We determine the equilibrium LC director field by minimizing Eq. (3) with respect to \( n(r) \) numerically as in Ref. \[9\].

We first discuss results obtained in the \( \lambda/\ell_e \ll 1 \) limit. Shown in Fig. 2 are the averaged pretilt angle of the calculated LC alignment at \( z = 0, \ \theta_{av}(0) \), plotted versus \( p \) for \( \lambda/\ell_e = 0.01 \) and various ratios of \( W_{\theta 1}/W_{\theta 2} \) from 0.5 to 5. As seen, all the curves in Fig. 2 bear similar shape with \( \theta_{av}(0) \) demonstrating a gentle rise from 6° as \( p \) increases from 0 initially, followed by an abrupt transition from small to high pretilt whereupon the rise with \( p \) becomes gradual again. For \( W_{\theta 1}/W_{\theta 2} = 1 \), the transition occurs at \( p = 1 \), but shifts to smaller (larger) \( p \) when \( W_{\theta 1}/W_{\theta 2} \) increases (decreases).

We plot \( \sigma_{\theta y}^2(z) \), the standard deviation of \( \theta(r) \) over the \( x-y \) plane at \( z \), against \( z \) for various \( \lambda/\ell_e \) from 0.01 to 1000 Fig. 3. In these plots, \( p = 0.125 \) and \( W_{\theta 1} = W_{\theta 2} \) though we found that the results are qualitatively independent of the set values of these parameters. As seen, when \( \lambda/\ell_e \ll 1 \ (= 0.01, 0.1) \), variations of the LC pretilt in the \( x-y \) plane is negligibly small for all \( z \), suggesting the director field to be uniform in the present limit. Hence the behaviors shown in Fig. 2 for LC alignment at \( z = 0 \) are essentially the same as those in the bulk. But
as $\lambda/\ell_e$ increases towards 1, $\sigma_\theta^{xy}(0)$ increases notably, and steadily approaches $\sim 27^\circ$ as $\lambda/\ell_e$ continues to increase towards 1000. We postpone discussion of the noted asymptotic value of $\sigma_\theta^{xy}(0)$ until later. Despite of the large variations in $\sigma_\theta^{xy}(0)$, all curves display similar decays towards 0 within $z = \lambda$. Least-square fittings reveal that the data of Fig. 3 can be described very well by exponential decays with decay lengths $\sim \lambda/2\pi$, consistent with previous results found in stripped surface patterns possessing zenithal inhomogeneity [3].

We return to the data of Fig. 2. In adopting an uniform LC director field, the system reduces the elastic energy in the expense of a larger surface energy. The resulting pretilt angle should then equal $\theta_{\min}$, the pretilt angle that minimizes the surface energy term of Eq. (3). It is straightforward to show that $\theta_{\min}$ satisfies:

$$\frac{1}{p} = 1 - \frac{W_{\theta 1} \sin 2(\theta_{\min} - \theta_{01})}{W_{\theta 2} \sin 2(\theta_{\min} - \theta_{02})}. \quad (4)$$

In Fig. 2 we plot $\theta_{\min}$ deduced from Eq. (4) versus $p$ for the same set of $W_{\theta 1}/W_{\theta 2}$ indicated in the figure (dashed lines). As seen, the data of $\theta_{\min}$ demonstrates excellent agreement with those of $\theta_{av}(0)$ obtained from simulations, verifying our interpretation that the uniform LC alignment is due to $\theta_{\min}$.

Next we consider the opposite limit where $\lambda/\ell_e \gg 1$. In this case, the director field on the surface is no longer uniform. But as Fig. 3 shows, it comprises large surface-induced deformations that decays to zero within a distance of $\sim \lambda/2\pi$ from the surface. Hence the homogenized LC alignment in the bulk could be obtained from that at $z = \lambda$. Shown in Fig. 4 are plots of $\theta_{av}(\lambda)$ versus $p$ for $\lambda/\ell_e = 1000$ and the same set of $W_{\theta 1}/W_{\theta 2}$ investigated in Fig. 2. In the same figure are drawn the corresponding data at $z = 0$ for comparison. As one could see, the average LC pretilts at both $z = 0$ and $z = \lambda$ are independent of $W_{\theta 1}/W_{\theta 2}$. It is interesting to note that the $z = 0$ data demonstrate a simple linear rise with $p$ from $6^\circ$ to $88^\circ$. This is because when $\lambda/\ell_e \gg 1$, the surface energy dominates the elastic energy in the LC system. One may thus assume that the LC director to exactly follow that of the local preferred direction of the anchoring surface, and hence $\theta_{av}(0)$ should just be the algebraic average of local preferred orientation over the surface, i.e., $p\theta_{01} + (1 - p)\theta_{02}$. If $p = 0.125$ as for the cases exemplified in Fig. 8 $\theta_{av}(0) = 16.25^\circ$. Then the standard deviation of $\theta(x, y)$ at $z = 0$ in the present limit would be $27.1^\circ$, in excellent accord with the value shown in Fig. 3 for $\lambda/\ell_2 = 1000$. The slightly larger value of $\theta_{av}$ in the bulk than that at $z = 0$ is attributable to the assumed $K_{33}$ being larger than $K_{11}$, which favors less bending in expense.
of more splay deformations of the LC director field in homogenizing into the bulk.

In this letter, we have considered in detail the pretilt alignment of nematic LC on a periodic patchy surface pattern comprising domains favoring either $88^\circ$ or $6^\circ$ zenithal alignments. If the pattern period is much smaller than the extrapolation length of the stronger anchoring domain, the LC alignment is uniform with the LC pretilt being one that minimizes the surface anchoring energy over one pattern period. But if the pattern period is much bigger than the extrapolation length of the stronger domain, the LC alignment at the interface copies the inhomogeneity of the surface pattern, which, however, dies out within one pattern period from the surface. The resulting homogenized LC zenithal alignment in the bulk is approximately given by the average of the local preferred directions of the domains weighted by their area fractions in the pattern. Previously Ong et al. created random inhomogeneous surfaces by depositing a discontinuous metal film on a silane (homeotropic agent) coated corrugated SiO$_2$ (homogeneous) substrate, then subjecting the sample to glow discharge to remove the silane unprotected by the metal islands, before dissolving the metal in the end. The average LC pretilt on these surfaces was found to increase monotonically from $0^\circ$ to $90^\circ$ as the average metal film thickness was increased, demonstrating good qualitative agreement with our results. Our results also display good consistency with those of Barbero et al. who obtained analytic solutions for LC alignment on stripped patterns favoring alternatively two dissimilar zenithal orientations (though the two preferred orientations must be sufficiently similar to validate their calculations). As most discussions presented here are general to LC alignment on inhomogeneous surfaces, it is probably that our results could be applicable to more general inhomogeneous patterns with irregular shapes. It is hoped that our study would motivate more experiments along the same line of thought.

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[1] E. Guyon, P. Pieranski, and M. Boix, Lett. Appl. Eng. Sci. 1, 19 (1973).

[2] D. W. Berreman, J. Phys. (France) 40, C3 (1979).

[3] G. Barbero, T. Beica, A. L. Alex-Ionescu, and R. Moldovan, J. Phys. II (France) 2, 2011 (1992).

[4] T. Z. Qian and P. Sheng, Phys. Rev. Lett. 77, 4564 (1996).

[5] H. L. Ong, A. J. Hurd, and R. B. Mayer, J. Appl. Phys. 57, 186 (1985).

[6] B. Lee and N. A. Clark, Science 291, 2576 (2001).

[7] J. Kim, M. Yoneya, and H. Yokoyama, Nature 420, 159 (2002).

[8] B. Zhang, F. K. Lee, O. K. C. Tsui, and P. Sheng, Phys. Rev. Lett. 91, 215501 (2003).

[9] O. K. C. Tsui, F. K. Lee, B. Zhang, and P. Sheng, Phys. Rev. E 69, 021704 (2004).

[10] F. K. Lee, B. Zhang, P. Sheng, H. S. Kwok, and O. K. C. Tsui, Appl. Phys. Lett. 85, 5556 (2004).
FIG. 1: Patterns used to simulate the inhomogeneous surface. Filled squares stand for the homeotropic domains; unfilled squares stand for the homogeneous domains. Periodic boundary conditions are imposed in the $x$ and $y$ directions.

FIG. 2: Simulation results of average pretilt angle $\theta_{av}(z = 0)$ versus $p$ for $\lambda/\ell_{e2} = 0.01$ and various $W_{\theta1}/W_{\theta2} = 0.5$ (crosses), 1.0 (triangles), 2.0 (diamonds) and 5.0 (squares) are shown. Dashed lines are the simulated $\theta_{min}$ versus $p$ according to Eq. 4 for the same set of $W_{\theta1}/W_{\theta2}$.

FIG. 3: Profiles of the standard deviation of the LC pretilt along $z$ for different ratios of $\lambda/\ell_{e2}$ from 0.01 to 1000. In these data, $p = 0.125$ and $W_{\theta1} = W_{\theta2}$.

FIG. 4: The average LC pretilt at $z = \lambda$, which is essentially the bulk value, versus $p$ for ($\lambda/\ell_{e2} = 1000$) for four different $W_{\theta1}/W_{\theta2}$ as indicated. The data for average pretilt at $z = 0$ are also drawn (solid line).
Fig. by Wan et al.
\[ \frac{W_{\theta_1}}{W_{\theta_2}} = 5.00 \]
\[ \frac{W_{\theta_1}}{W_{\theta_2}} = 2.00 \]
\[ \frac{W_{\theta_1}}{W_{\theta_2}} = 1.00 \]
\[ \frac{W_{\theta_1}}{W_{\theta_2}} = 0.50 \]

Fig. 2 by Wan et al.
Fig. 3 by Wan et al.
$\theta_{av}(0)$

- $W_{\theta 1}/W_{\theta 2} = 5.00$
- $W_{\theta 1}/W_{\theta 2} = 2.00$
- $W_{\theta 1}/W_{\theta 2} = 1.00$
- $W_{\theta 1}/W_{\theta 2} = 0.50$

Fig. 4 by Wan et al.