LIQUID CRYSTAL PHASE TRANSITIONS INDUCED BY MICRO-TEXTURED SUBSTRATES

Tie-Zheng Qian[†] and Ping Sheng

Department of Physics, The Hong Kong University of Science and Technology,
Clear Water Bay, Kowloon, Hong Kong

Abstract—Through a numerical approach based on the Landau-de Gennes theory, we show that novel orientational states and phase transitions may be induced in nematic liquid crystals by micro-textured substrates, i.e., spatially mixed homeotropic, planar, or homogeneous alignment potentials.

I. INTRODUCTION

Properly treated substrate can induce preferential bulk alignment in liquid crystals (LC). Most of the prior studies have been focused on uniform substrates. Perfectly uniform substrates are rare, however, and conventionally by uniform substrates one usually means those samples where the micro-structure scale is much shorter than the LC elastic correlation length. When the typical scale of the substrate is comparable to the intrinsic LC correlation length, novel orientational states are expected. There have been some prior works which examined the effective alignment induced by inhomogeneous substrates [1-3]. However, due to the use of the Frank-Oseen elastic distortion free energy as the theoretical framework, the spatial variation of the order parameter close to the surface was neglected. In addition, the elastic correlation length in the Frank-Oseen theory is essentially infinite [4], so the substrate inhomogeneities are effectively homogenized. The purpose of this paper is to show the crucial role of a finite elastic correlation length in the bulk alignment induced by textured substrates with spatially mixed alignment boundary conditions. Through a Landau-de Gennes approach, we find that for a stripe pattern of alternating planar and homeotropic aligning conditions there can be a first order phase transition between two bulk orientational states in which one has the director lying in the yz plane, where z is normal to the substrate and

y is parallel to the stripes, and the other one aligned along the x -direction, shown schematically in Fig. 1.

II. LANDAU-DE GENNES FORMALISM

Consider a half space $z \geq 0$ where the substrate, defined to be at $z = 0$, is textured into a periodic stripe pattern in the x direction with alternating stripes having either a homeotropic aligning potential, given by $G_n Q_{33} \delta(z)$, or a planar aligning potential, given by $G_p Q_{33} \delta(z)$ [5,6]. Here $G_n \leq 0$, $G_p \geq 0$ are the surface potential constants, and Q_{33} is the zz -component of the symmetric, traceless tensor order parameter Q_{ij} , with the correspondence $1 \leftrightarrow x$, $2 \leftrightarrow y$, and $3 \leftrightarrow z$. Here we consider only the case where the alternating stripes have equal width, with a periodicity P . To determine the liquid crystal configuration(s) resulting from the surface alignment potentials, we use the Landau-de Gennes free energy expression [7] as the basis of our calculation. In the absence of externally applied field, the total free energy F of the system may be written in the dimensionless form as

$$\Psi = \frac{F}{\Delta^3 B^4 / C^3} = \Psi_B + \Psi_S, \quad (1)$$

where the bulk free energy Ψ_B and the surface free energy Ψ_S are given by

$$\begin{aligned} \Psi_B = \int d^3\zeta \quad & \left(t + \frac{1}{4} \right) \left(\frac{2}{3} \bar{Q}_{ij}^2 \right) - \frac{4}{3} \bar{Q}_{ij} \bar{Q}_{jk} \bar{Q}_{ki} + \left(\frac{2}{3} \bar{Q}_{ij}^2 \right)^2 \\ & + \frac{2}{3 + 2\rho} \bar{Q}_{ij,k}^2 + \frac{2\rho}{3 + 2\rho} \bar{Q}_{ij,j} \bar{Q}_{ik,k}, \end{aligned} \quad (2)$$

$$\Psi_S = \int d^3\zeta [g(\zeta_1) \bar{Q}_{33} \delta(\zeta_3)]. \quad (3)$$

Here $\bar{Q}_{ij} = C Q_{ij} / B$, the length unit $\Delta = \sqrt{LC/B^2}$ is the elastic correlation length, which characterizes the distance over which the order parameter can vary significantly, $t = (T - T_c) / 4(T_c - T^*)$ with $4(T_c - T^*) = B^2 / aC$ being the temperature unit, $\rho = L_2 / L_1$, and

[†] Permanent address: Institute of Theoretical Physics, Beijing 100080, P. O. Box 2735, People's Republic of China

Fig. 1. Schematic illustration of the textured stripe pattern with alternating homeotropic and planar alignment conditions. The directors of the two bulk orientational states are shown at right.

Fig. 2. The director configurations of the yz state and the x-state in the transition layer.

the material constants a, B, C, L are those associated with the usual Landau-de Gennes free energy density f in the uniaxial case, where S is the orientational order parameter: $f = a(T - T^*)S^2 - BS^3 + CS^4 + L(\partial S/\partial z)^2$. T_c and T^* have the usual meanings of the nematic-isotropic phase transition temperature and the supercooling temperature, respectively, and $L = (3L_1/4) + (L_2/2)$. The dimensionless surface constant g is noted to be a function of x . Its unit is given by $G = \Delta B^3/C^2$. For 5CB, $a=0.065\text{J}/\text{cm}^3\text{K}$, $B=0.53\text{J}/\text{cm}^3$, $C=0.98\text{J}/\text{cm}^3$, $L = 4.5 \times 10^{-14}\text{J}/\text{cm}$, and $\rho \simeq 1$ [5]. Accordingly, we have $\Delta = 40\text{\AA}$, $G = 0.614\text{erg}/\text{cm}^2$, and the temperature unit is 4.4K . The values of $g_n = -0.05$ and $g_p = 0.08$ are used here [8].

Mean-field equilibrium state is given by the order parameter configuration which minimizes the free energy functional. To obtain the configuration $\bar{Q}_{ij}(\vec{z})$ which minimizes the total free energy Ψ , we use the fourth-order finite difference scheme to discretize the derivatives and employ the conjugate gradient method to seek the optimal configuration.

III. PHASE TRANSITIONS

Every nematic liquid crystal has an intrinsic elastic correlation length on the order of Δ . When $P \geq 10\Delta$, we obtain the so-called yz state as the bulk configu-

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Fig. 3. Variation of the tilt angle θ , measured from the xy plane, and the azimuthal angle ϕ , defined relative to the x-axis, plotted as a function of substrate texture periodicity P at fixed $t = -1.0$. Solid line denotes the θ variation; dashed line denotes the ϕ variation. The dotted line denotes the tilt angle variation of the metastable yz state. A first order phase transition is noted at $P = 47.3\Delta$.

ration, together with a transition boundary layer of thickness proportional to P , as illustrated in Figs. 1 and 2. The bulk director lies in the yz plane because the twist elastic constant is smaller than the bend and splay elastic constants. At fixed temperature, as P decreases, the bulk director's tilt angle θ decreases continuous to zero at some finite value of P . However, before it can reach zero, a first-order transition occurs and the bulk director jumps from the yz plane to x axis, as depicted in Fig. 3. The director configuration of the so-denoted x state is illustrated in Figs. 1 and 2. If P is fixed not far away from 50Δ , the same transition can be observed by varying the temperature around $t = -1.0$ because the elastic correlation length is temperature-dependent. For fixed $P = 47.5\Delta$, a first order-transition occurs at $t = -1.017$, as depicted in Fig. 4, with an entropy change of $\Delta s = 9.17 \times 10^{-5} a \Delta B^2/C^2$. It is seen that the x state is characterized by very small distortion in the boundary layer and a very larger surface energy in the homeotropic region of the substrate. In essence, the transition is from an elastic-energy dominated yz state to a surface-energy dominated x state. Why the alignment is along the x axis rather than the y axis is intriguing at first sight. We find the $\bar{Q}_{ij,j}\bar{Q}_{ik,k}$ term in Ψ_B , which breaks the rotational symmetry about the z axis, is actually responsible. Due to the finite value of θ around the transition point, at either above or below the first-order transition, it is possible to have a field-induced first-order transition provided the dielectric anisotropy $\delta\epsilon_a$ is negative or positive. We consider the nematic liquid crystal to be in a cell of thickness D , sandwiched between two similarly textured substrates. For $D = 6\mu\text{m}$, $t = -1.0$, $P = 50\Delta$, $\delta\epsilon_a \simeq -0.1$, a field-induced switching from the yz-state to the x state occurs as the applied voltage

Fig. 4. Variation of the tilt angle θ , plotted as a function of temperature t for fixed $P = 47.5\Delta$. The dotted line denotes the tilt angle variation of the metastable yz state. A first order phase transition is noted at $t = -1.017$.

exceeds 3 volts.

It should be of interest to investigate other possible orientational states and phase transitions that can be induced by different micro-texturings. What we present here only serves to illustrate the possibilities associated with a new class of substrates and their induced effects.

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