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Effect of phase shift between geometrical and chemical patterning in nematic liquid crystal cells: A Monte Carlo study

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ABSTRACT

Thin films of nematic liquid crystals confined to geometrically as well as chemically patterned substrate at one end and a planar substrate with strong anchoring at the other are studied employing non-Boltzmann Monte Carlo methods. We investigate the effect of temperature on the director structures as the system goes through the isotropic-nematic phase transition. The low temperature results show significant deviations from the phase diagram predicted within the continuum approximation, depicted as a function of the tilt angle at the top substrate and the thickness of the cell. Onset of phase biaxiality is observed at very low temperatures, and it increases as the tilt angle at the top substrate is increased, moving away from the normal to the substrate. A phase shift introduced between the geometrical and chemical patterns at the other end also enhances the phase biaxiality of the system to a fairly high value. This seems to provide a convenient experimentally tunable parameter for controlling the symmetry of the director structures.

1. Introduction

Nematic liquid crystals in contact with solid substrates are extensively used in display devices, like the twisted nematic configurations between flat substrate surfaces. The application of a small external field is sufficient to change qualitatively the equilibrium director configurations dictated by the substrates, and thus leading to profound changes in the optical properties of the nematic cell. Surface inhomogenities could occur as a natural result of surface treatments like rubbing, needed to induce the desired boundary conditions. However such inhomogenities do not reflect in the bulk properties of the nematic cell as long as the length scales of the surface patterns are very small compared to the thickness of the cell as well as to the wavelength of the visible light. More recent developments however have demonstrated that surfaces patterned with large periodicity are of considerable interest from technological point of view like, for example, in flat panel displays with wide viewing angles ([1] and references therein). In view of their potential technological importance, it is essential to examine the anchoring effects in detail, and investigate possible transitions between different equilibrium director structures induced by non-uniform surface interactions. Moreover, these systems could prove to be very interesting if they were to be found to exhibit bistable nematic states with different director orientations possible at the same energy [2–6]. Whereas many experimental and theoretical studies have concentrated on either geometrically [7,8] or chemically patterned surfaces [9–13], nematic liquid crystals confined to both geometrically structured and chemically patterned substrates have been objects of investigation only recently [14–17]. For example, studies based on the continuum theory of nematic liquid crystals in contact with specific geometrically and chemically patterned substrates predicted transition between two nematic director structures, the so-called H and HAN phases [14,15,17], on varying the thickness of the cell or changing the anchoring angle, θ_D at the top substrate as depicted in Fig. 1. In such studies, the interaction of the nematic liquid crystal system in contact with sinusoidal grating with alternating patterns of homeotropic and planar anchoring is accounted for, based on the Frank–Oseen model for distortion free energy [18,19], while the surface energy function is written in terms of the Rapini–Papoular interaction [20].

Theoretical treatments normally proceed by reducing the dimensionality of the system for convenience of analysis, taking into account the translational invariance along one of the directions, and sometimes by performing a conformal mapping appropriately to eliminate one more dimension. Further, a planar surface inducing an effective anchoring angle is assumed to mimic

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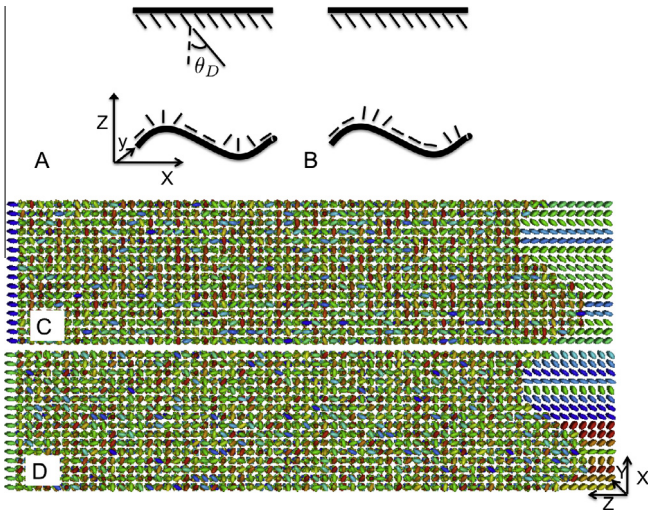

Fig. 1. *Liquid crystal cell:* (A and B) Schematics of liquid crystal cell with both geometrical and chemical patterns applied in-phase and shifted by *pi*/8 respectively. The head-less vectors indicate the molecular orientations at the grated substrate. The liquid crystal molecules at the top substrate are oriented at tilt angles θ_D ranging from 0° to 45°. (C and D) Snap shots of the initial configuration of liquid crystal cell of Model A and Model B respectively. The colour code indicates the relative orientations of the molecules with respect to the *Z*-direction. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the geometrical pattern at the grooved substrate [14–17]. The underlying argument relies on the observation that the effect of the patterned surface does not extend into the film beyond the length scale of the geometric structure and hence can be replaced by an effective free energy expansion. In all the cases the equilibrium configurations under different distorting conditions are obtained by minimizing the effective free energy functional so proposed.

The rationale for these simplifications could have been the prohibitive effort involved in tackling the problem more exactly through numerical procedures within continuum approximation. Such an extremization procedure under the stated simplifications *inter alia* however does not allow for possible role of thermal effects which are indeed important in real nematic samples. Simulations also provide additional advantage of following the thermal behaviour of the system through its IN transition. Keeping these merits in view, we perform Monte Carlo simulations of the model liquid crystal system based on inter-molecular interactions among the molecules given by Lebwohl–Lasher potential [21], imposing suitable boundary conditions to mimic geometrical as well as chemical patterns. We employ entropic sampling techniques [22,23,25] to investigate this confined system, as has been recognized earlier to be crucial for such studies [27].

In this article, we implement a specific geometrical and chemical pattern which has been recently investigated analytically via free energy minimization procedure, and study the effect of relevant control parameters on the formation of the film as the temperature is cooled, looking for stable structures at very low temperatures. We also examine the onset of phase biaxiality by introducing a phase shift between geometrical and chemical patterns in the nematic liquid crystal cell.

2. Model and simulation methodology

Lebwohl–Lasher potential [21] describing the interaction between two nearest neighbouring liquid crystal molecules placed on a cubic lattice is given by:

$$H = -\sum_{\langle i,j \rangle} \epsilon_{ij} P_2(cos(\theta_{ij})) \quad (1)$$

Here, $\epsilon_{ij} = \epsilon$ if two nearest neighbours at i and j are liquid crystal molecules; $\epsilon_{ij} = \omega$, the anchoring strength, if one of the nearest neighbours is a substrate molecule and ω varies between 0 and 1. The summation $\langle i,j \rangle$ is over all the nearest neighbours in the lattice. The top layer is a solid substrate inducing strong anchoring at an angle, θ_D with respect to the homeotropic direction, as shown in Fig. 1. A sinusoidal pattern is carved out of the bottom layers (say, with amplitude, A) along the x-axis. The thickness of the cell, D along the z-direction is taken to be large compared to the amplitude of the sinusoid. The surface induced interaction is invariant along the y-direction. We choose the cell thickness to be much larger than the period of the sinusoidal grating, P at the bottom surface, and the amplitude of the sinusoid to be smaller than its wavelength. Now, in order to implement this scenario on a lattice model, we choose a cubic lattice of size $16 \times 16 \times 66$, in the notation of x, y and z dimensions shown in Fig. 1. We introduce a sine wave extending over 16 lattice points in the x-dimension, and a film thickness (z-direction) of 66 units. While the y-dimension could be argued to be unimportant within the continuum approximation (since the problem under simplifying assumptions is reducible to x–z plane), simulating at microscopic level necessitates extension into the y-dimension. Accordingly, we consider the system to extend over 16 lattice units in this direction as well. We find that it has some interesting consequences on the development of bistability of the system. Periodic boundary conditions are applied along the x and y directions. The amplitude of the sinusoidal grating was initially chosen to be 8 units. Such a choice may not implement accurately the geometrical constraints implied in [16], due to the limitations introduced by the discretization of space into lattice; it does however capture essential features of the underlying model. The crucial assumption in the continuum treatment is that any arbitrary distribution of the anchoring direction over the grating period is essentially taken into account by introducing an effective tilt angle (say, $\theta_{a_{eff}}$) for purposes of predicting the bulk behaviour of the film. The focus of this simulation is thus more on the process of formation of the director structures as the nematic phase forms, as well as the realizability of phase biaxiality and its tuning by introducing a phase shift between geometrical and chemical patterning of the substrates at low enough temperatures.

We consider two model systems in the present work based on the phase shift introduced between the chemical and geometrical patterns on the bottom substrate, see Fig. 1A and B. In Model A, the chemical pattern is in-phase with the geometrical pattern. Homeotropic alignment is induced at crests and troughs of the sinusoidal wave each for a period of one fourth of the period of geometrical sine wave, while in the other regions locally planar alignment is imposed. In Model B, the chemical pattern is shifted by one-eighth of the wavelength with respect to the geometrical pattern in contrast to Model A. The anchoring directions in the two models are shown in Fig. 1A and B. Initial configurations of the liquid crystal cell in both the models are illustrated in Fig. 1C and D. Each ellipsoid represents the collective orientation of a group of liquid crystal molecules positioned at that lattice point. Their relative orientations with respect to the z-direction are colour coded in the figures: blue colour represents molecules parallel to z-axis while red represents perpendicular to the z-axis. We employ modified frontier sampling method [23] to study the system for different angles, θ_D in the nematic region. We compute the density of states (DoS) and hence collect entropic ensemble of microstates fairly uniformly distributed with respect to the system energy. We then extract the canonical ensemble at any desired temperature by appropriate re-weighting procedure [24]. Thus for each value of θ_D, we compute equilibrium averages of different