Director structures with dominant in-plane alignment in hybrid planar films of biaxial nematic liquid crystals: A Monte Carlo study

B. Kamala Latha [a,*], G. Sai Preeti [a,1], K.P.N. Murthy [a,2], V.S.S. Sastry [a,b]

[a] School of Physics, University of Hyderabad, Hyderabad 500046, India
[b] School of Engineering Sciences and Technology, University of Hyderabad, Hyderabad 500046, India

ABSTRACT

Equilibrium director structures in two thin hybrid planar films of biaxial nematics are investigated through Markov chain Monte Carlo simulations based on a lattice Hamiltonian model within the London dispersion approximation. While the substrates of the two films induce similar anchoring influences on the long axes of the liquid crystal molecules (viz. planar orientation at one end and perpendicular, or homeotropic, orientations at the other), they differ in their coupling with the minor axes of the molecules. In Type-A film the substrates do not interact with the minor axes at all (which is experimentally relatively more amenable), while in Type-B, the orientations of the molecular axes at the surface layer are influenced as well, by their biaxial coupling with the surface. Both films exhibit expected bending of the director associated with the ordering of the molecular long axes due to surface anchoring. Simulation results indicate that the Type-A film hosts stable director structures in the biaxial nematic phase of the LC medium, with the primary director lying in the plane of the film. High degree of this stable order thus developed could be of practical interest for potential applications. Type-B film, on the other hand, experiences competing interactions among the minor axes due to incompatible anchoring influences at the bounding substrates, apparently leading to frustration.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

The biaxial nematic phase (N_B) of liquid crystals (LC), predicted theoretically very early [1], and realised experimentally in the past decade, in bent-core [2–4], tetrapode [5–7], and polymeric [8,9] systems, is characterised by a primary director $\boldsymbol{n}$ and a secondary director $\boldsymbol{m}$ (perpendicular to $\boldsymbol{n}$). Field-induced switching of the secondary director is envisaged to be faster than the primary director in the biaxial nematic phase, a fact which endows these nematics with a promising potential for use in fast switching electro-optic devices [10,11]. The orthorhombic N_B phases with D_{2h} symmetry are suggested to be desirable [12] for ready applications.

While the current experimental studies are still concerned with unambiguous confirmation of macroscopic biaxiality [12–14], theoretical studies have been more optimistic. Modelling the Hamiltonian in terms of interactions among molecular tensors, mean-field predictions within quadratic approximation envisage systems

which condense into liquid crystal phases with biaxial symmetry [15–19]. These encompass molecular structures with wide ranging symmetry [20]. Computer simulations [21] on the other hand have been playing a significant role in investigating these models systematically. Recent Monte Carlo studies based on this lattice model focus on the competing effects of different energy contributions in the Hamiltonian on the ordering of the medium [22–24] in biaxial systems. A molecular dynamics (MD) simulation of the bulk biaxial Gay-Berne fluid under the action of an electric field [25] has convincingly shown that the switching of the director, associated with the minor molecular axes, is an order of magnitude faster than that of the director defined by the long molecular axes.

In the biaxial nematic phase, a different pathway for fast switching between different birefringent states (compared to conventional uniaxial LC systems) is possible because the birefringence can be changed by a rotation of the short axes which are thermally ordered, while the orientation of the long axes could be kept fixed [26]. A possible device configuration to achieve this objective is to use a film of biaxial liquid crystal confined in a planar cell with hybrid boundary conditions, wherein the geometry could constrain the orientation of the primary director (of the long axes) in the biaxial nematic phase, leaving the secondary director (of one of the short axes) free for switching with an appropriate


(in-plane) field. Studies on uniaxial hybrid films have established [27,28] that a bent-director configuration could be realised if the film thickness is greater than a critical thickness determined by the curvature elasticity of the medium and the surface interaction strength. Preliminary work on their biaxial counterpart was carried out earlier [29].

In this context, we investigated the equilibrium director structures in two planar films of biaxial liquid crystals, in the uniaxial and biaxial phases of the medium. The anchoring influences of the two substrates comprising the cell are used to pin the orientation of the primary director [ordering direction of the major (long) axes of the molecules] near the two surfaces so as to result in a bent-director hybrid structure. The substrates can be chosen either not to have influence on the minor axes of the molecules (pure uniaxial coupling with the substrate, say Type-A film), or to couple with the minor axes as well (biaxial coupling with the substrate, say Type-B film). We simulated director structures in both these films based on Markov chain Monte Carlo (MC) sampling technique, constructing corresponding equilibrium ensembles. This paper reports our results examining the role of different anchoring conditions on the orientational ordering in the medium for potential applications.

In Section 2 we introduce the lattice model of the medium, and details of the anchoring conditions of the two films. The MC simulation are also discussed in this section. The equilibrium director structures of the film in the two nematic phases obtained from the computations are depicted and discussed in Section 3. We also examine the effect of varying the cell thickness, as well as of the relative anchoring strengths at the two substrates, on the director structures in these films. The last section summarizes our conclusions.

2. Model and simulation details

We consider a planar hybrid film comprising of LC molecules with D_{2h} symmetry. We assign the right-handed triad $\{X, Y, Z\}$ to represent the laboratory-fixed frame and $\{x, y, z\}$ to represent the molecular-fixed frame. We let z direction represent the molecular long axis, while the other two (minor) axes are represented by y and x. The film is obtained by confining the biaxial molecules between two planar substrates taken to be in the X–Y plane. Fig. 1 shows the schematics of a biaxial molecule, orienting influences at the two substrates of the planar film, and the reference axes of the laboratory. The orientational interactions between LC molecules, relevant to the present study, are conveniently accounted for, by adopting a lattice Hamiltonian model wherein the molecules located at the lattice sites are represented by unit vectors in the $\{x, y, z\}$ frame specifying the individual molecular orientations. Within this lattice description, in a film of thickness d the substrate planes are positioned at $Z = 0$ and $Z = d + 1$ (lattice units). The influence of the substrates is simulated by introducing two bounding layers of molecules contained in these planes with the designated, but fixed, orientations, referred to in the literature as ghost molecules [30]. The anchoring conditions in both the films are such that the long axes of the molecules are hybrid-aligned (planar orientation parallel to say, Y-axis at one substrate and homeotropic at the other, parallel to Z-axis). For adequately thick films, the primary director $\boldsymbol{n}$ is bent satisfying the two incompatible boundary conditions. We distinguish two scenarios: (a) in Type-A film, the ghost molecules interact with the LC molecules in the surface layer anchoring only their long axes, thus implying that the substrate hosts only cylindrically symmetric rod-like LC constituents, and (b) in Type-B film the ghost molecules themselves have D_{2h} symmetry and interact through a Hamiltonian model appropriate to the biaxial system. These correspond to
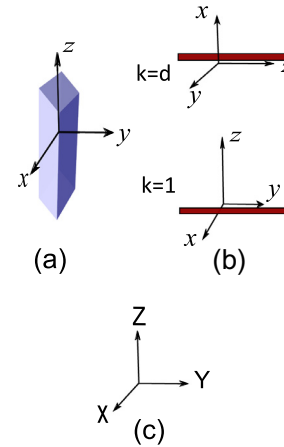
Fig. 1. Schematic illustrations of (a) typical biaxial molecule (b) anchoring directions at the two substrates of the film: homeotropic at the lower ($k = 1$) substrate and planar at the top ($k = d$) (c) orientation of the laboratory frame relative to the film.

two qualitatively distinct chemical treatments of the anchoring substrates.

In Type-A film, the molecular z-axes are anchored along the Z-direction in the surface layer near, say, the lower substrate of the cell ($k = 1$), while they are kept planar (say, parallel to Y-axis) in other surface layer, near the substrate ($k = d$). As the substrates do not interact with the minor axes of the molecules in this film, they are not, *a priori*, oriented in any specific direction, until guided to equilibrium conditions by the intermolecular and substrate interactions.

In the Type-B film, we impose anchoring conditions of equal strength on all the three molecular axes at each of the two substrates, and use the biaxial Hamiltonian model to account for their interactions with the substrates. The boundary conditions on the film at the two surfaces are summarized as (see Fig. 1):

Substrate 1 at $Z = 0 : z\|Z, y\|Y, x\|X$
Substrate 2 at $Z = d + 1 : z\|Y, y\|Z, x\|X$

2.1. Model Hamiltonian

The biaxial LC molecules are assumed to interact through a pairwise additive lattice Hamiltonian within the London dispersion approximation [31], expressed in terms of generalised Wigner rotation matrices as:

$$U(\omega_{ij}) = -\epsilon_{ij}\left\{P_2(\cos(\beta_{ij})) + 2\,\lambda_d\left[R_{02}^2(\omega_{ij}) + R_{20}^2(\omega_{ij})\right] + 4\,\lambda_d^2\,R_{22}^2(\omega_{ij})\right\} \quad (1)$$

where $\epsilon_{ij} = \epsilon$ sets the energy scale, and is used to define the reduced temperature, $\omega(\alpha, \beta, \gamma)$ is the set of Euler angles which specify the rotations to be performed in order to bring the reference frame of two molecules i and j in coincidence, R_{mn}^2 are symmetrized Wigner functions, $P_2(\cos(\beta_{ij}))$ is the second Legendre polynomial and λ_d quantifies the biaxial interaction between the molecules. The average values of R_{mn}^2 define the order parameters of the medium in the nematic phases. These are: the uniaxial order $\langle R_{00}^2 \rangle$ (along the primary director), the phase biaxiality $\langle R_{20}^2 \rangle$, and the molecular contribution to the biaxiality of the medium $\langle R_{22}^2 \rangle$, and the contribution to uniaxial order from the molecular minor axes $\langle R_{02}^2 \rangle$ [31]. For simulation purposes, the above Hamiltonian is recast in the Cartesian form, as