Applicability of hybrid planar films of biaxial nematics for in-plane switching: A detailed Monte Carlo study.

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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 ordering of the molecular long axes due to surface anchoring. Simulation results indicate that the Type - A film hosts stable and noise free director structures in the biaxial nematic phase of the LC medium, resulting from dominant ordering of one of the minor axes in the plane of the substrates. High degree of this stable order thus developed could be of practical interest for in-plane switching applications with an external field. 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, and hence to noisy equilibrium director structures.
I. 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 $n$ and a secondary director $m$ (perpendicular to $n$). 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], computer simulations [15] on the other hand have been playing a significant role in the investigation of biaxial systems. A molecular dynamics (MD) simulation of the bulk biaxial Gay-Berne fluid under the action of an electric field [16] has convincingly shown that the switching of the secondary director is an order of magnitude faster than the switching of the primary director.

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 [17]. 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 [18, 19] 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 also carried out earlier [20].

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 biaxial anchoring on the orientational ordering in the medium, and looking for their suitability to utilize the secondary director for possible switching applications.

In section II 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 III. 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.
II. 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 are located at the lattice sites represented by unit vectors $\{x, y, z\}$ 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 \[21\]. 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 $n$ 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 cylindrical 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 two qualitatively distinct chemical treatments of the anchoring substrates.
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.

In Type - A film, the molecular z-axes are anchored along the Z-direction in the surface layer near, say, 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 by equilibrium conditions under a given interaction model.

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 is summarized as (see Fig. 1):
Substrate 1 at Z=0 : \( z \parallel Z, y \parallel Y, x \parallel X \)

Substrate 2 at Z=d+1 : \( y \parallel Z, x \parallel Y, z \parallel X \)

A. Model Hamiltonian

The biaxial LC molecules are assumed to interact through a pair-wise additive lattice Hamiltonian [22] within the London dispersion approximation, expressed in terms of generalised Wigner rotation matrices as:

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

where \( \epsilon_{ij} = \epsilon \) sets the energy scale, and is used to define the reduced temperature, \( \omega(\alpha, \beta, \gamma) \) are 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, \( R_{mn}^L \) are symmetrized Wigner functions, \( P_2(\cos(\beta_{ij})) \) is the second Legendre polynomial and \( \lambda_d \) quantifies the biaxial interaction between the molecules. The average values of \( R_{mn}^L \) define the order parameters of the medium in the nematic phases. These are: the uniaxial order \( < R_{00}^2 > \) (along the primary director), the phase biaxiality \( < R_{20}^2 > \), and the molecular contribution to the biaxiality of the medium \( < R_{22}^2 > \), and the contribution to uniaxial order from the molecular minor axes \( < R_{02}^2 > \) [22].

For simulation purposes, the above Hamiltonian is recast in the cartesian form, as

\[
U = -\epsilon \left\{ \frac{3}{2} V_{33} - \sqrt{6} \lambda_d (V_{11} - V_{22}) + \lambda_d^2 (V_{11} + V_{22} - V_{12} - V_{21}) - \frac{1}{2} \right\}.
\]
Here, $V_{ab} = (u_a \cdot v_b)^2$, and the unit vectors $u_a, v_b, [a, b = 1, 2, 3]$, are the three axes of the two interacting neighbouring molecules. $\lambda_d$ sets the relative importance of the biaxial interaction in the Hamiltonian, while $\epsilon$ (set to unity in the simulations) defines the temperature scale ($T' = \frac{k_B T^*}{\epsilon}$), where $T^*$ is the laboratory temperature in Kelvin.

This model in a bulk system was studied extensively both through mean-field analysis and MC simulations based on Boltzmann sampling methods. The value of $\lambda_d$ for the present study is kept at 0.35, keeping in view the high degree of biaxiality it induces, as well as the convenience of a wider biaxial nematic range of temperature made available for our study [22].

**B. Simulation Details**

A planar hybrid film of (lattice) dimensions $15 \times 15 \times d$ ($d = 6, 8, 10, 12$ layers) is considered in the present work. Periodic boundary conditions are applied along the laboratory X and Y directions, so as to minimize finite size effects. The anchoring conditions applied at the two substrates (contained in the X-Y plane) depend on the specific choice of the film (Type A or B), and their relative strengths are chosen as desired. We index the LC layers with $k$, starting from the substrate imposing homotropic anchoring influence on the long molecular axes. The LC ghost molecules in the substrate layers (which are adjacent to the two bounding layers of the LC medium) do not participate in the Monte Carlo dynamics. The interaction strengths of the long molecular axes at the two substrates are represented by $\epsilon_1$ and $\epsilon_d$, and $\epsilon_d$ can be varied relative to $\epsilon_1$ (which is set equal to 1). The temperature $T'$ (in dimensionless units) is set by the coupling strength $\epsilon$ in the Hamiltonian (Eqn.1).

In each simulation, the reduced temperature is varied from 2 to 0.05 in steps of 0.005, and at each temperature the film is equilibrated for $5 \times 10^5$ lattice sweeps.
FIG. 2: Variation with temperature of system properties a bulk biaxial film (15 × 15 × 15): specific heat $C_V$ peaks mark the phase transitions $I - N_U$ and $N_U - N_B$. Uniform growth of the order parameters major order parameters $R_{00}^2$, $R_{22}^2$ can be observed.

(Attempted moves over all the sites), while the data from the resulting canonical ensembles are collected over a production run of $5 \times 10^5$ lattice sweeps. The physical properties computed are the average values of energy $E$, the specific heat $C_v$, the order parameters $R_{00}^2$, $R_{02}^2$, $R_{20}^2$, $R_{22}^2$ [23] as well as their susceptibilities, and layer-wise orientation of the local directors (orientation averaged over the layer) with respect to the laboratory Z-axis (polar angle $\theta$, layerwise) as well as the angle made by the local layer-wise director with respect to laboratory X-axis (azimuthal angle $\phi$, layerwise). We computed both layer-wise properties (to examine the director structure and its relative changes) as well as the film properties (averaged over the sample), as a function of temperature, for a fixed relative anchoring strength and layer thickness. The simulations are then repeated by varying the thickness effecting the length scale of the system, and also varying the anchoring strength ($\epsilon_d$) to look for possible anchoring-induced transitions among the different director structures.
III. RESULTS AND DISCUSSION

Fig. 2 depicts the variation of specific heat and the major order parameters in a bulk biaxial fluid (without confinement) of dimensions (15×15×15) computed based on MC simulations under periodic boundary conditions, using the above dispersion Hamiltonian model at $\lambda d=0.35$. The two peaks in the specific heat at $T_1 = 1.123$ and $T_2 = 0.571$ indicate the high temperature $I-N_U$ and low temperature $N_U-N_B$ phase transitions [22]. The phases, as identified by the Metropolis-based Boltzmann sampling procedure employed here, are marked by uniform growth of the uniaxial order $R_{00}^2$ and the biaxial order $R_{22}^2$, as a function of temperature, bringing out the onset of the uniaxial phase $N_U$ and low temperature biaxial phase $N_B$. Fig. 3 shows their variation in the Type - A film. Fig. 4 provides variation of all the four order parameters and their susceptibilities in Type - A film, averaged over the sample. The qualitative difference between the thermal evolution of these order parameters in the bulk and Type - A film (in particular $R_{00}^2$) may be noted for further discussion later. The director structure in the film is better appreciated by examining the degree of ordering in each layer and the orientation of the local layer director with respect to laboratory axes, specified by their $\theta$ and $\phi$. These layer-wise properties are shown for Film-A in Fig. 5. Similar data were obtained for Film-B as well, and are represented in Figs. 6 - 8 respectively. It is to be noted that layer-wise angles of the local directors are obviously not meaningful in the isotropic phase, and hence such information in these figures (Figs. 5 and 8) (generated automatically during computations) are to be ignored. Such data are relevant only in the ordered phases and are subject of our discussion.
FIG. 3: Variation with temperature of system properties in Type - A film. Specific heat \( C_V \) peaks mark the phase transitions \( I \rightarrow N_U \) and \( N_U \rightarrow N_B \). The bent - director structure of uniaxial order parameter \( R_{00}^2 \) in the uniaxial phase and the increase in biaxial order \( R_{22}^2 \) in the uniaxial phase itself, are attributed to effects of geometric confinement.

A. Type - A Film

We note at the outset that in this film the substrate interacts with only the long axes of the molecules, while LC molecules themselves have biaxial interaction among them. This system undergoes two transitions at \( T_1 = 1.021 \), and the second at \( T_2 = 0.525 \), exhibiting the sequence \( N_B \rightarrow N_U \rightarrow I \) (see Fig. 3). It is observed that both transition temperatures are lowered, in comparison with the those in a bulk sample (see Fig. 2).

Figs. 4(a) and 4(b) show the four order parameters of the system along with their susceptibilities. It is observed from Fig. 4(a) that the \( R_{00}^2 \) susceptibility profile, which is a measure of the fluctuations in the long-range order of the primary director, shows two peaks. The larger peak (at \( T_1 \)) corresponds to rapid increase of \( R_{00}^2 \) in the uniaxial nematic phase. The \( R_{00}^2 \) curve displays a bent-director structure and attains a maximum value of 0.6 in this phase. The smaller peak close to \( T_2 \) signals a sudden change in the slope of the \( R_{00}^2 \) curve leading to a steady increase of the
dominant (uniaxial) order towards a maximum value of unity deep in the biaxial phase. The susceptibility of the biaxial order, on the other hand, shows a single broad peak at a temperature slightly higher than $T_2$, signalling the onset of biaxial order in this phase. The non-zero value of $R_{22}^2$ at the onset of the $I - NU$ transition itself is attributed as due to the geometric confinement (cf. Fig. 2 of bulk system).

Contribution to the ordering along the uniaxial director originating from molecular minor axes, $R_{02}^2$ and the phase biaxiality parameter arising from the non-cylindrical distribution of the molecular long axes around the primary director, $R_{20}^2$ are shown in Fig. 4(b). As compared to their values in a bulk system, we observe that these parameters have non-zero values in the uniaxial nematic phase, - a clear manifestation of the geometric confinement.

The layer-wise variations (for the layer index $k = 1$ to $d$) of properties connected with director structures, plotted along with the corresponding bulk values of the film (sample averages) are shown in Figs. 5(a) - 5(c). It is observed from Fig. 5(a)
FIG. 5: Layer-wise variation of different properties of the Type A film, with temperature: (a) $R_{20}^2$ and $R_{22}^2$ (b) $R_{02}^2$ and $R_{20}^2$ (c) Angle $\theta$ and Angle $\phi$ (see text).
that layer-wise $R_{00}^2$ values vary smoothly, unlike the abrupt jump at $T_2$ exhibited by the sample average. Further, the order values in all the layers asymptotically reach the maximum value of 1.0 at the lowest temperature. The variation also shows that the middle layers ($k = 4$ and 5), being the least influenced by the substrate boundaries, are most effective in contributing to the critical onset of the order at the transition. The sample average and layer-wise behaviour of biaxial order shows that in the middle layers $R_{22}^2$ starts increasing from the $I - N_U$ transition itself, but a significant increase is observed only at the $N_U - N_B$ transition. The layer-wise $R_{02}^2$ and $R_{20}^2$ are shown in Fig. 5(b). It is observed that they have small, but non-zero values in the uniaxial nematic phase in the middle layers of the film.

The plots of the layer-wise $\theta$ (angle made by the layer-wise director with respect to the laboratory Z-axis) and layer-wise $\phi$ (angle made by the layer-wise director with respect to the laboratory X-axis) are shown in Fig. 5(c). Focusing on the data only below the clearing point, it is observed that as the temperature is lowered from the isotropic phase, layer-wise $\theta$ values stabilise at certain fixed values in the nematic phase. The value of this angle increases monotonically from $k = 1$ layer to the $k = d$ layer, clearly indicating that the layer-wise primary director bends gradually from the lower substrate to the upper substrate, corresponding to the expected bent-director structure. The layer-wise $\phi$ angles show a sudden flip by approximately 90° just below the $I - N_U$ transition, particularly in the region of middle layers, pointing to the onset of a long-range order, essentially confining the primary director to the laboratory YZ plane, as the system is cooled. The profile of the layer-wise angle also suggests that this bent-director structure is not affected by the $N_U - N_B$ transition.
FIG. 6: Variation with temperature of system properties in Type-B film - peaks of the specific heat $C_V$ mark the phase transitions $I - N_U$ and $N_U - N_B$. The phases are identified by the growth of the major order parameters $R_{00}^2$ and $R_{22}^2$.

B. Type-B Film

Introduction of biaxial coupling between the substrates and the surface film layers, in the presence of an already constrained bent primary director, introduces incompatible boundary conditions on the minor axes as well, and seem to lead to some curious manifestations.

Referring to Fig. 6 it may be noted that the onset of biaxial order in Type-B film occurs only at the $N_U - N_B$ transition unlike the case of Type - A film. Further, Figs. 7(a) and 7(b) show that all order parameter susceptibilities, except that of $R_{22}^2$, display appreciable fluctuations in the biaxial phase, and these are reflected on their (average) order profiles as well.

The system and layer-wise variations of different order parameters are shown in Figs. 8(a) - 8(b). The layer-wise $R_{00}^2$ values in Fig. 8(a) do not fluctuate in the biaxial phase and attain maximum ordering, interestingly unlike the system order parameter. The layer-wise biaxial order shows a non-zero value just below the $I - N_U$ transition and grows gradually, whereas the system biaxial order develops
appreciably only at the $N_U - N_B$ transition. Both fluctuate significantly in the biaxial phase similar to the other order parameters. The layer-wise $R_{02}^2$ and $R_{20}^2$ shown in Fig. 8(b) have small, nonzero values in the uniaxial nematic phase, but show similar fluctuations in the biaxial phase.

The layer-wise $\theta$ and layer-wise $\phi$ values shown in Figs. 8(c) depict variations with temperature in the two nematic phases, which are largely similar to the behaviour of Type - A film, but for significant fluctuations on the onset of the $N_U - N_B$ transition. It appears that the layer-wise magnitudes of the two dominant orders are relatively stable, but their orientations are not.

We now discuss the evolution of the uniaxial sample order ($R_{00}^2$) in the two films as the system transits through the two transitions, specifically in comparison with the layerwise behaviour (Figs. 5(a), 8(a)). Focussing on Type - A film initially, we note that the sharp increase in this order at the second $N_U - N_B$ transition is unlike the
FIG. 8: Layer-wise variation of different order parameters of the Type-B film, with temperature: (a) $R^2_{00}$ and $R^2_{22}$ (b) $R^2_{02}$ and $R^2_{20}$ (c) Angles $\theta$ and $\phi$ (see text).
FIG. 9: Type - A film (a) Variation of maximum eigen values ($q_{max}$) associated with each of the ordering tensors of the three molecular axes ($x$, $y$, $z$), as a function of temperature (b) The orientations of the corresponding eigen vectors plotted as a function of the Monte Carlo steps after equilibration, at temperature $T = 0.5$ below the $N_U - N_B$ transition temperature.

variation in the bulk sample (Fig. 2), and is not supported by its layer-wise variations. The latter are smoothly varying across the transition, and the director angles ($\theta$, $\phi$) also do not betray the presence of an intermediate phase transition. And yet, the bulk order of the film, defined and computed as corresponding to the maximum eigen value of the ordering tensors of the three molecular axes, is very sensitive to this transition. The case of the Type - B film is qualitatively the same, but for the onset of significant fluctuations in the $N_B$ phase at $T_2$. This points to the need to further investigate this system in terms of thermal variations of the eigen values of the three axes separately and examine their behavior across this transition.

Accordingly, we computed equilibrated averages (over the film) of the maximum eigen values ($q_x$, $q_y$, $q_z$) of the ordering tensors ($Q_{xx}$, $Q_{yy}$, $Q_{zz}$) of the three molecular
FIG. 10: Type - B film :(a) Variation of maximum eigen values ($q_{\text{max}}$) associated with each of the ordering tensors of the three molecular axes ($x, y, z$), as a function of temperature; (b) The orientations of the corresponding eigen vectors plotted as a function of the Monte Carlo steps after equilibration, at temperature $T = 0.5$ below the $N_U - N_B$ transition temperature.

axes and depict their variation for the case of Type - A film in Fig. 9(a). We also show the directions ($\theta, \phi$) of the corresponding three eigen vectors, as a function of MC steps after equilibration, in the $N_B$ phase, in Fig. 9(b). From these two figures, it is evident that the onset of the biaxial phase in this confined system (at $T_2=0.5$) leads to a sudden change in the direction of dominant order of the film itself. While the alignment of the long molecular axes defines the primary director till $T_2$, it is the molecular $y$ axes which are the most ordered among the three, below this temperature. In conjunction with Fig. 9(b), we see that the ordering direction of this calamitic axis is indeed in the laboratory X-direction in the biaxial phase, while the other two eigen vectors are confined to the laboratory YZ plane, mutually perpendicular to each other. It may be noted that the onset of a biaxial phase thus
leads to maximal ordering of the second major axes, wholly contained in the plane of the substrate, and the anchoring conditions imposed in this case constrain only the long axes of the LC molecules, along with the minor $x$-axes of the molecules.

In contrast, Type - B film which imposes anchoring restrictions on the minor axes of molecules as well at both the ends, presents a very different scenario. We refer to Fig. 10(a) showing $(q_x, q_y, q_z)$ as a function of temperature in this film. At the onset of the second transition (at $T_2 \sim 0.51$), $q_z (\sim 0.617)$ is higher than the $q_x (\sim 0.536)$ and $q_y (\sim 0.447)$. However on further cooling, $q_x$ crosses the value of $q_z (\sim 0.632$ at $T' = 0.433$), while $q_y$ remains less than $q_z$. At lower temperatures $q_x$ saturates at $\sim 0.87$, while $q_y$ and $q_z$ saturate to a value of $\leq 0.72$. Eigen vector of $q_z$ makes an angle $\theta \sim 45^0$ with the laboratory Z-direction and $\phi \sim 90^0$ with laboratory X-direction, thereby indicating that the bent-director structure originating from the ordering of the molecular $z$-axes is contained in the YZ plane, as is also the case in the high temperature nematic phase. Curiously the eigen vector of $q_y$ is oriented at angles $\theta \sim 45^0$ and with a fluctuating $\phi$ varying between $0^0$ to $90^0$ (see Fig. 10(b)).

The maximal ordering direction in this film is determined by the ordering tensor of the molecular $x$-axes and its azimuthal angle $\phi$ is eventually contained in the plane of the substrate pointing to the laboratory X-direction. It may be noted that the corresponding fluctuations of the azimuthal angle $\phi$ of the local directors of the $x$ and $y$ molecular axes are complementary (Fig. 10(b)).

It is thus obvious that the observed significant noise in the thermal averages of $R^2_{00}$, $R^2_{20}$ and $R^2_{02}$ at the onset of the $N_B$ phase arises due to the fluctuations in the directions of the different ordering tensors (Figs. 7(a) and 7(b)). The relative stability observed in the case of $R^2_{22}$ (in the $N_B$ phase) perhaps follows from the interesting circumstance that the biaxial order in this film is defined by the ordering of the molecular $y$ and $z$ axes; while the ordering direction of the $z$ axes is fairly stable, that of $y$ axes fluctuates however complementary to the primary director defined by the
molecular $x$ axes. The qualitatively different scenario of the Type - B film, relative to Type - A, arises due to the imposition of additional restrictions on all the molecular axes at the two substrates.

Comparing the two films in their biaxial phase, we observe that both have primary director (defined as the direction of maximum molecular order) contained in the plane of the substrates, with molecular $y$-axes defining such a direction for the Type - A film while $x$-axes play that role for Type - B film. However, imposition of anchoring constraints on all molecular axes leaves the second film frustrated, leading to significant fluctuations of the ordering directions. Moreover from a practical point of view, it is much easier to prepare substrates which need to restrain only one type of axes of the system. Thus Type - A lends itself as a possible structure containing stable and significant order contained within the plane of the film (and hence can be unambiguously coupled to an in-plane external field), with the added convenience in the preparation of required substrates.

C. Effect of thickness in a Type - A film

Because of its simplicity and stable structures, we examined the effect of varying the thickness $d'$ in the Type - A film, ($d = 6, 8, 10, 12$ lattice units), while retaining the same lateral dimensions, and anchoring strengths at the two substrates. Fig. 11 shows this effect on the specific heat $C_V$ and Figs. 12(a) and 12(b) depict the consequent changes in $R_{00}^2$, $R_{22}^2$, $R_{02}^2$ and $R_{20}^2$, respectively.

It is observed that the specific heat profiles become sharper as the thickness increases (size effect). The uniaxial order parameter $R_{00}^2$ increases marginally in the uniaxial phase as the thickness increases, retaining its bent director structure for all thickness. The biaxial order $R_{22}^2$ shows a slight decrease as the thickness increases and shows a marked increase in the temperature of the nematic phase itself for a
FIG. 11: Comparison of variations of the specific heat $C_V$ as a function of temperature in films of thickness $d$ (in lattice units) = 6 (stars), 8 (circles), 10 (upward triangles) and 12 (diamonds), in Type - A film.

FIG. 12: Comparison of variation of different order parameters with temperature in Type - A film for different film thickness ($d$). (a) $R_{00}^2$ and $R_{22}^2$; (b) $R_{02}^2$ and $R_{20}^2$; $d = 6$ (stars), $d = 8$ (circles), $d = 10$ (upward triangles) and $d = 12$ (diamonds), in Type - A film.

A thinner film ($d=6$). The $R_{02}^2$ and $R_{20}^2$ values decrease as the thickness increases (size effect). These observations indicate that the gross features of director structures in Type - A film are relatively insensitive to the film thickness, alluding to some degree
FIG. 13: Variation of order parameters with temperature for different anchoring strengths ($\epsilon_{nz}$) in Type A film of thickness 6 lattice units: (a) $R_{00}^2$ and $R_{22}^2$ (b) $R_{02}^2$ and $R_{20}^2$.

D. Effect of anchoring strength in Type - A film

We further examined the Type - A film (at fixed thickness $d = 6$) with respect to a change in the anchoring strength $\epsilon_d$ at the surface layer. We relax the strong anchoring condition ($\epsilon_d = 1$) and vary its value now from 0.0 to 0.6 in steps of 0.1, and compute equilibrium averages (as a function of temperature) of the four order parameters. We depict their dependence on $\epsilon_d$ in Fig. 13. The other simulative conditions remain the same as before.

We observe from Figs. 13(a) and 13(b) that for anchoring strengths $\epsilon_d=0.0$ (no anchoring influence at the top substrate) and for a low value of $\epsilon_d = 0.1$, the uniaxial
order $R_{00}^2$ and the biaxial order $R_{22}^2$ attain maximum values of 1.0 and 0.5, respectively; for example without the characteristic features observed earlier (with $\epsilon_d = 1$) at the onset of the $N_B$ phase. Their variations are similar to bulk LC systems without confining surfaces (see Figs. 2 and 3). For $\epsilon_d \geq 0.2$ the primary director assumes a bent structure and the primary order is constrained with an upper bound of 0.8 for $\epsilon_d = 0.2$ in the uniaxial nematic phase. A similar sharp difference is exhibited by $R_{22}^2$ as well, and its temperature variation qualitatively changes above the threshold value of $\epsilon_d = 0.2$. The order parameters $R_{02}^2$ and $R_{20}^2$, shown in Fig. 13(b), start with very low values at $\epsilon_d = 0.0$ and 0.1, but increase significantly for higher anchoring strength ($\epsilon_d \geq 0.2$). Thus it appears that a minimum threshold anchoring strength ($\epsilon_d \geq 0.2$) is necessary for the film to exhibit the curious structures, described earlier, arising from the bent formation of its director. The progressive development of this scenario with increase of $\epsilon_d$ is evident from the gradual decrease of the system primary order (Fig. 13(a)) in the uniaxial phase.

IV. CONCLUSIONS

Equilibrium director structures in thin planar films of biaxial LC medium, imposing hybrid boundary conditions at the two substrates on the molecular long axes (z-axes), are investigated through Monte Carlo simulation, based on a Hamiltonian model under dispersion approximation (at $\lambda_d = 0.35$). Boltzmann sampling is adopted which corresponds to the established phase sequence involving uniaxial and biaxial phases ($N_B - N_U - I$) in bulk samples. Two different films were considered: Type - A in which only the long axes are anchored at the substrates and Type - B in which all molecular axes are suitably anchored. Very interestingly, Type - A film leads to a stable, noise free, high order parameter value for $R_{00}^2$ deep in the biaxial phase region, and this order is due to the near perfect alignment of the molecular
\(y\)-axes in a direction perpendicular to the plane hosting the bent director structure associated with the long molecular axes. This scenario is appealing for two reasons: the Hamiltonian model is realistic as it accommodates both the perturbing interactions (the last two terms in Eqn.1), and secondly the substrates are needed to influence suitably only the long molecular axes, which is more practical. Under these convenient conditions we find that in the biaxial phase, one can generate an in-plane order of high degree involving one of the minor axes of the molecules, while the bent director from the anchored alignment of the long axes is conveniently locked within the plane perpendicular to this dominant order. Type - A film appears to be a good candidate for further studies of switching with external in-plane fields. Type - B film on the other hand is frustrated on entering into the biaxial phase, apparently due to the competing energetic demands of different contributions to the Hamiltonian arising from incompatible surface anchoring influences involving the minor axes.

The effect of the variation of the thickness is marginal. The Type - A film seems to undergo an anchoring-induced transition in its director structures when the \(\epsilon_d\) is tuned. These two observations could to be useful inputs in designing a practical device with switchable in-plane order.

In summary, we conclude that the Type - A film, involving realistic LC biaxial molecular system with simple hybrid anchoring conditions imposed only on the long axes is a potential candidate to generate a high degree of in-plane order in the biaxial phase, amenable for coupling to external fields.

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