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Effect of Surface Anchoring on Creation of Defects in a Nematic Film. A Monte Carlo Simulation

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Nematic systems confined to a bounded volume are particularly interesting because they present stable structure defects induced by the anchoring conditions on the surface. Here we present a Monte Carlo study of a hybrid nematic film with various strengths of coupling with the surfaces.

Keywords Monte Carlo; Hybrid nematic film; boundary conditions; anchoring; defects

Introduction

Hybrid nematic films have received a great deal of attention, both for their application in display technology and for their fundamental interest concerning the behavior of mesophases in a restricted environment [1]. It is well known that defects appear in nematic films with hybrid boundary conditions when the film thickness h is much smaller than its lateral size L. Such stable defects for this liquid crystal (LC) system have been investigated experimentally and on the basis of continuum theory [2] as well as by lattice spin simulations [3]. In particular we have shown in the past that Monte Carlo simulations can reproduce the appearance of stable point defects in a hybrid nematic system with a certain thickness to surface area ratio and suitable boundary conditions, i.e. where the spins of the bottom layer, $z = 0$, have random fixed orientations in the horizontal (X, Y) plane, while those of the top layer, $z = h$, are homeotropically oriented, i.e. fixed along the surface normal [3].

It is also known that discilination lines can be formed in a perfect hybrid nematic cell where the two flat surfaces enclosing the nematic are, like before, perpendicular to the surface at $z = h$ but aligned uniformly along X or Y at $z = 0$ [4]. The surface boundary conditions will tend to influence the orientation of molecules near to the surface and the

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aligning effect may propagate inside the film. In general there will be a competition between the molecular orientation induced by surface boundary condition, the effects of ordering on the liquid crystal itself due to the molecules trying to arrange parallel to each other, and the disordering effect of temperature. The resulting molecular organization for a certain boundary condition will thus depend on a number of factors, including the strength of the surface interaction, the temperature and so on. We have shown that Monte Carlo simulations can be a particularly effective tool to predict the combined result of these factors [5].

Here we wish to study by Monte Carlo (MC) simulations the influence that the anchoring energy, i.e. the strength of the coupling with the surfaces have on the formation of defects in the case of the hybrid nematic film where the surfaces has a perpendicular alignment. We have chosen to use the Gruhn-Hess-Romano-Luckhurst (GHRL) pseudopotential [6, 7] which takes into account the elastic anisotropies to investigate the problem.

We have already shown that the model is suitable for simulating the optical textures of thin uniaxial films with random planar (schlieren) and hybrid conditions for a number of cases with various elastic constant anisotropies [8, 9] and here we use the same approach to monitor the results.

The Simulation Model

The Gruhn-Hess-Romano-Luckhurst model [6, 7] consists of a system of interacting centers ("spins") placed at the sites of a certain regular lattice, here taken as cubic. The Hamiltonian is written as follows:

$$U_N = (1/2) \sum_{\substack{i,j \in F \\ i \neq j}} \Phi_{ij} + J_t \sum_{\substack{i \in F \\ j \in S_t}} \Phi_{ij} + J_b \sum_{\substack{i \in F \\ j \in S_b}} \Phi_{ij} \tag{1}$$

where F, S_t, S_b are the set of particles in the bulk and at the top and bottom surfaces, respectively, and the parameter J_t models the strength of the coupling with the top surface and J_b the anchoring with the bottom one. The particles interact through the second rank attractive pair potential:

$$\begin{aligned} \Phi_{jk} = \varepsilon_{\mathrm{jk}} \{ & \lambda [P_2(\mathbf{u_j} \cdot \mathbf{s}) + P_2(\mathbf{u_k} \cdot \mathbf{s})] + \\ & \mu [(\mathbf{u_j} \cdot \mathbf{s})(\mathbf{u_k} \cdot \mathbf{s})(\mathbf{u_j} \cdot \mathbf{u_k}) - 1/9] + \nu P_2(\mathbf{u_j} \cdot \mathbf{u_k}) + \\ & \rho [P_2(\mathbf{u_j} \cdot \mathbf{s}) + P_2(\mathbf{u_j} \cdot \mathbf{s})] P_2(\mathbf{u_j} \cdot \mathbf{u_k}) \} , \end{aligned} \tag{2}$$

where $\varepsilon_{jk} = \varepsilon$ for nearest neighbors and zero otherwise, is a dimensionless parameter which determines the interactions strength and

$$\begin{aligned} \lambda &= (1/3)\, \Lambda\, (2\mathrm{K}_1 - 3\mathrm{K}_2 + \mathrm{K}_3) ; \\ \mu &= 3\Lambda\, (\mathrm{K}_2 - \mathrm{K}_1) ; \\ \nu &= (1/3)\, \Lambda\, (\mathrm{K}_1 - 3\mathrm{K}_2 - \mathrm{K}_3) ; \\ \rho &= (1/3) \Lambda\, (\mathrm{K}_1 - \mathrm{K}_3) \end{aligned}$$

with K_1, K_2, K_3 the splay, bend and twist elastic constants. Λ is a factor which, for dimensional consistency, has the dimension of a length. The vectors $\boldsymbol{s}$ and $\boldsymbol{r}$ are defined as follows: $\boldsymbol{s} = \boldsymbol{r} / |\boldsymbol{r}|$, $\boldsymbol{r} = \boldsymbol{x_j} - \boldsymbol{x_k}$, with $\boldsymbol{x_j}$, $\boldsymbol{x_k}$ dimensionless coordinates of the j-th and k-th lattice points. $\boldsymbol{u_j}$, $\boldsymbol{u_k}$ are unit vectors along the axis of the two particles ("spins") and P_2 is a second rank Legendre polynomial. Notice that the pair potential eq. 2, although it has formally the same mathematical structure of the Lebwohl-Lasher one [10], is temperature

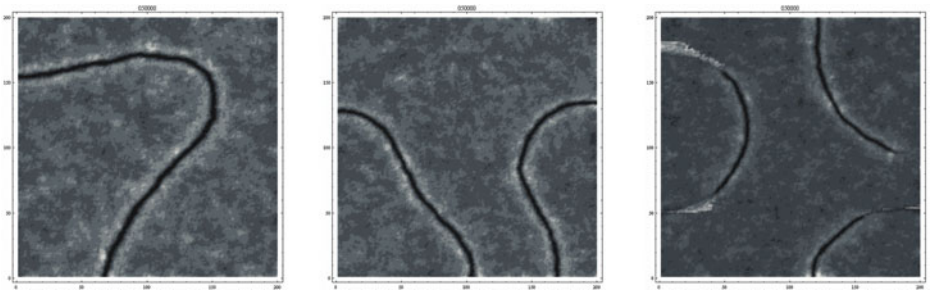

Figure 1. Simulated optical images as obtained by MC simulations of a 200 × 200 × (10 + 2) GHRL film system with homeotropic alingnment at the top and alignment along X at the bottom. At the four lateral faces FBC were employed. The elastic constants are those of 5CB and the coupling with the surfaces are equal, i.e. $J_t = J_b = 0.3, 0.4, 0.5$ from left to right respectively.

dependent through the elastic constants K_i. In the one constant approximation ($K_1 = K_2 = K_3$) as a special case, i.e. $\lambda = \mu = \rho = 0$, it reduces and, a part this hidden temperature dependence, to the simple Lebwohl-Lasher (LL) potential.

We have considered a 200 × 200 × (10 + 2) system with each surface boundary condition implemented with the help of an additional layer of particles, kept fixed during the simulation, with orientations chosen to mimic the desired alignment at the top and at the bottom of the film. Empty (free, FBC) or periodic boundary conditions (PBC) are employed at the other four lateral faces of the system.

We present results obtained using elastic constants correspondent to typical values for 5CB at a temperature well inside the nematic phase, i.e. $K_1 = 7.0 \times 10^{-12}$ N, $K_2 = 4.4 \times 10^{-12}$ N, $K_3 = 9.7 \times 10^{-12}$ N [11], but we can anticipate that the main observations are similar for the Lebwohl-Lasher model, i.e. in the one constant approximation. This suggest that the results are due mainly to the surface boundary conditions, at least for the elastic constants of 5CB. The starting configurations of the lattice are chosen with the spins completely aligned along the Z direction and the evolution of the system is followed while it proceeds according to the classic Metropolis Monte Carlo procedure [12] reorienting one spin at a time, so as to ensure proper equilibration.

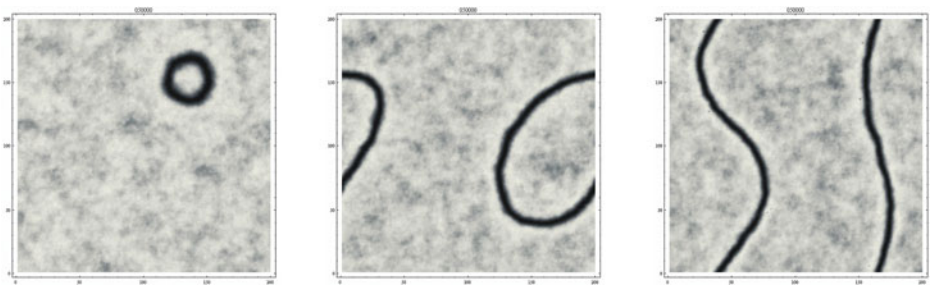

Figure 2. Simulated optical images as obtained by MC simulations of a 200×200× (10+2) GHRL film system with homeotropic alignment at the top and planar alignment along the diagonal of the XY plane at the bottom. At the four lateral faces PBC were employed while the other simulation parameters are the same of those of Fig. 1 with $J_t = J_b = 0.3, 0.4, 0.5$ from left to right respectively.

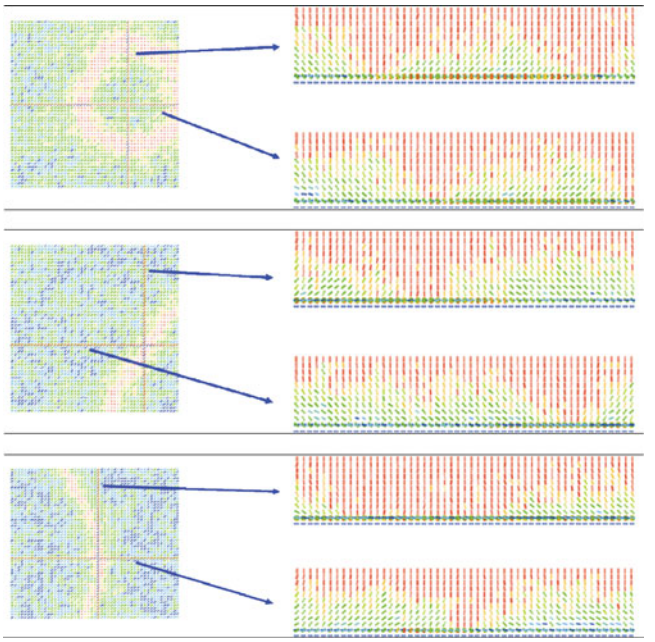

Figure 3. Snapshots of the middle layer (left side) and two vertical cuts, positioned as indicated by the arrows, (right side) of regions where the disclinations occur and corresponding to portions of the images in Fig. 2. The color code indicates the spin orientations with the red one denoting the alignment along Z.

Simulations and Results

We have performed a set of independent simulations at a temperature $T^* = kT/\varepsilon = 0.4$ for various values of the couplings J_t and J_b. The Monte Carlo results have been used to simulate images corresponding to those observed with polarized light microscopy, an experimental technique used to investigate micrometer size films, starting from the simulated lattice configurations by means of a well established matrix approach [13, 14]. We describe each site in the nematic film as an optical retarder represented by a Müller matrix, so that the light beam travelling through a succession of sites across the layers of the system is retarded by the matrix resulting from the product of the Müller matrices corresponding to each site. The light emerging from the film is observed, when required, with the help of crossed polarizers (45 and 135 degrees) placed on each side of the cell, which are represented by appropriate projection matrices and switch off the non retarded light. Finally the light intensity emerging from the cell is coded in a scale from black (no light) to white (full intensity) with 32 different grey levels.

We present in Fig. 1 three optical images obtained by Monte Carlo simulations for three different values of coupling with the surfaces where the spins are fixed and aligned along Z at the top and along X at the bottom and for the case of equal anchoring strength for the two surfaces. The lateral boundary conditions are chosen free (FBC) in this case as mentioned before.

We can notice the appearance of disclination lines. These are due to the particular alignments at the film surfaces which, in the case of planar and aligned orientation at the bottom tends to favour the creation of disclination lines. On the contrary, it is well

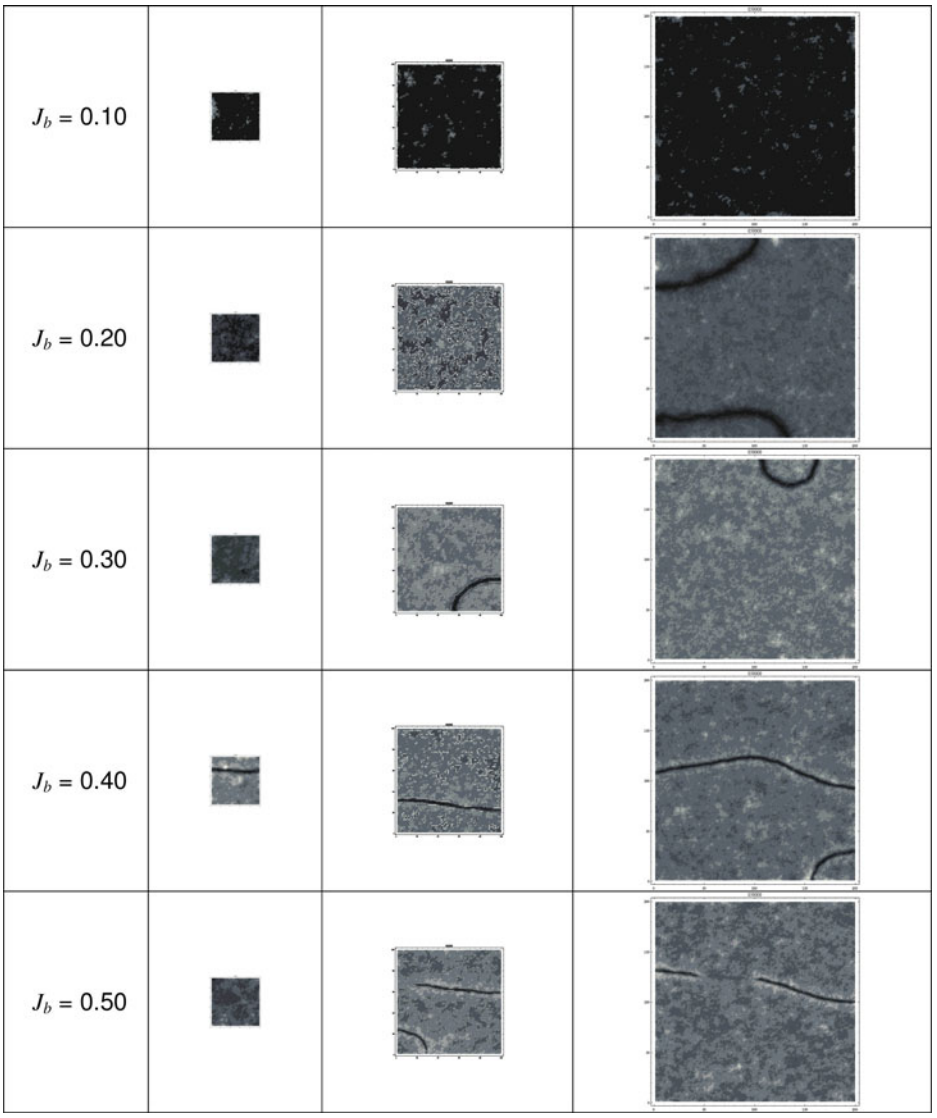

Figure 4. Simulated optical images as obtained by MC simulations of nematic films with homeotropic alingnment at the top and uniform alignment along X at the bottom. At the four lateral faces FBC were employed. The elastic constants are those of 5CB and the coupling with the surfaces are $J_t = 1$ and various values of J_b. We present results corresponding to three system sizes, i.e. $50 \times 50 \times (10 + 2)$, $100 \times 100 \times (10 + 2)$ and $200 \times 200 \times (10 + 2)$ and polarizers at 45° and 135°.

known that if at the planar boundary of the hybrid film a random organisation is imposed, this favours the appearance of stable point defects [3]. Moreover, we can see that these disclination lines seem to become thinner as the anchoring with the surfaces increases.

This result becomes more evident (see Fig. 2) when considering an alignment at the bottom surface along the diagonal so to have the same angle (45 degrees) of one polarizer and lateral PBC. In this case the images are clearer and brighter and the PBC seem to enhance the effect of the film surfaces. In Fig. 3 we can appreciate the molecular organization at the

defect zone by looking at the snapshots plotted using different colors for the various spin orientations.

As mentioned before the creation of disclination lines corresponds to a uniform alignment at the bottom surface. We have then also tried to investigate the case, maybe more interesting from the technical and experimental point of view, of strong homeotropic anchoring at the top, which is realized for example for 5CB at a nematic-air interface, while a weaker ordering coupling is present at the bottom.

It seems that a stronger bottom anchoring should move the wall closer to the top surface. As a consequence the weaker anchoring produces a more dark texture (Fig. 4). This expectation can be understood with a sharp change of director orientation in a thin hybrid film with strong anchoring, as predicted by Barbero and Barberi [15] and Palffy-Muhoray [16]. These predictions have been confirmed by atomistic simulations of 5CB on crystalline silicon H-terminated [17], where, however, the sample is very small (only a few nm) and no texture can be observed along X,Y.

A particularly interesting feature of the present results, shown in Fig. 4 for three different system sizes and for some values of the bottom coupling J_b, is that they seem to confirm also in this case that the disclination line is thinner when the anchoring is stronger.

This observation may be considered from a phenomenological perspective. It is well known that, in the one constant approximation, the elastic energy (F) of a uniform hybrid aligned nematic cell is given by

$$\mathrm{F} = \pi K\, h\alpha^2 R^2 / \,2,$$

where K is the elastic constant, h is the thickness of the sample, R is the lateral size of the system, and $\alpha = (\theta_b - \theta_t)/\, h$, with θ_b and θ_t representing the angles between **n** and the normal to the bottom and top surfaces, respectively [18]. The presence of a disclination line contributes to the total energy with a term of the kind KR. Moreover, a surface contribution should be also considered.

Similarly to the surface energy of a point defect which is of the form $F_c \sim W\, {r_c}^2$ a rough estimation of that contribution yields $F_c \sim W\, r_c\, R$, where W is the anchoring energy whereas r_c is the defect core size. This term has been estimated considering the disclination formed as a sequence of N point defects along a straight line, thus N is of the order of $R\,/\,r_c$. It is then clear that when W increases, the lines become thinner for optimizing the energy of the system.

Conclusions

We have performed Monte Carlo simulations of hybrid aligned nematic films with varying the strengths of the coupling with the confining surfaces. Our simulations are based on the lattice parametrization of the Gruhn-Hess-Romano-Luckhurst potential which takes into account the main elastic constants and that was already used to investigate then confined liquid crystals. In our calculations we have used values of the elastic constants corresponding to those typical of 5CB. The main results are the expected creation of disclination lines which are favoured by the alignment along X and Z respectively at the bottom and top surfaces. In addition the thicknesses of these lines seem to be related to the strength of the anchoring at the planar aligning surface.

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