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Effect of Surface Orientation on Director Configurations in a Nematic Droplet. A Monte Carlo Simulation

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Abstract We present a Monte Carlo study of a nematic droplet with boundary conditions that vary from an homeotropic to a bipolar anchoring. We follow the change in the molecular organisation inside the droplet as the boundary conditions vary by calculating order parameters and experimental observables like Deuterium NMR line shapes and polarized microscopy textures.

Keywords Monte Carlo, Polymer dispersed liquid crystals, boundary conditions, defects.

INTRODUCTION

Polymer dispersed liquid crystals (PDLC) have received a great deal of attention, both for their applications in display technology and for their fundamental interest concerning the behavior of mesophases in a restricted environment [1]. These materials consist of nematic droplets embedded in a polymer matrix where the molecular organization in the liquid crystal can be strongly influenced by the boundary conditions at the droplet surface. The surface boundary conditions will tend to influence the orientation of molecules near to the surface and the aligning effect will tend to propagate inside the droplet. In general there will be a competition between the molecular

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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 in predicting the combined effect of these factors [2]. Nematic systems confined in a restricted volume are also interesting because they present stable structure defects induced by the anchoring conditions on the surface [3]. A particular interesting case is where the boundary conditions vary from an homeotropic to a bipolar anchoring [4]. When changing the surface tilt angle from homeotropic to planar anchoring there is a continuous change from a configuration with a radial point defect to a bipolar configuration with surface defects at the poles of the drop. Here we wish to investigate this case by computer simulations on a lattice spin model.

THE SIMULATION MODEL

The Monte Carlo simulations were based on a simple Lebwohl - Lasher spin model [5]. The droplet is approximated by a roughly spherical sample S obtained from a cubic lattice by considering all the molecules falling within a given distance from the chosen center. The particles interact through the attractive nearest neighbours Lebwohl - Lasher pair potential and the different boundary conditions are mimicked assuming a layer of outside particles G with a fixed orientation determined by the specific type of boundary condition [6]. Thus the model hamiltonian is:

$$U_{i,j} = \begin{cases} -\varepsilon_{ij} P_2(\cos\beta_{ij}) & \text{for } i,j \in S \\ -\varepsilon_{ij} J P_2(\cos\beta_{ij}) & \text{for } i \in S,\ j \in G \end{cases} \qquad (1$$

where ε_{ij} is a positive constant, ε, for nearest neighbours particles i and j and zero otherwise, β_{ij} is the angle between the axis of the two molecules, P_2 is a second rank Legendre polynomial and J determines the strength of coupling to the external environment. The spins

represent a cluster of neigboring molecules whose short range order is maintained through the temperature range examined [7].

As we have mentioned before, in this work we have considered boundary conditions that vary from a perfect radial (hedgehog) configuration to a bipolar one. To take into account this variation we have introduced the angle θ between the boundary spin orientation, which lies on the meridian plane crossing the sphere at that point, and the local normal to the surface. Then the angle θ ranges from $\theta = 0^\circ$ (radial) to $\theta = 90^\circ$ (bipolar).

The updating of the lattice configurations is done according to a standard Metropolis Monte Carlo procedure [8], reorienting one spin at a time, so as to ensure proper equilibration.

SIMULATIONS

We have performed a set of independent simulations at a temperature $T^* = kT/\varepsilon = 0.4$ for various values of the tilt angle, i.e. $\theta = 0^o, 5^o, 10^o, 15^o, 20^o, 30^o, 40^o, 50^o, 60^o, 70^o, 80^o$ and 90^o. The droplet is carved from a $22 \times 22 \times 22$ latttice and the number of particles (spins) inside the sample was set to 4272 whereas the additional surface layer fixing the boundary conditions contains 1128 spins. We used the potential in eq.1 with anchoring strength $J=1$ in all cases. We calculate in particular energy, U, and second and fourth rank order parameters, $\langle P_2 \rangle_\lambda$ and $\langle P_4 \rangle_\lambda$ obtained from the largest eigenvalue of the ordering matrix. The approximate lattice droplet is divided in concentric shells making it is possible to calculate the relevant physical quantities going from the center of the sphere to the surface. Moreover we have used the Monte Carlo configurations to simulate polarized light microscopy images and to calculate polydomain deuterium NMR line shapes, which are observables directly accessible from real experiments [4,9]. The polarized optical textures, experimentally used to investigate micrometer size droplets, can be obtained from the simulated lattice configurations by means of a standard matrix approach [6,10]. We describe each site in the droplet by a Müller matrix, so that the light beam travelling through a row 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 retarded by the spins in the droplet is observed, when required, with the help of crossed polarizers placed on each side of

the cell, which switch off the non retarded light and are represented by appropriate projection matrices. 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.
The other experimental observables obtained from the simulated configurations are the Deuterium NMR line shapes calculated for a system of fictitious molecules with an axis of effective molecular uniaxial symmetry [11]. Here diffusion effects [12] are neglected and every line shape is an average obtained from a set of different configurations.

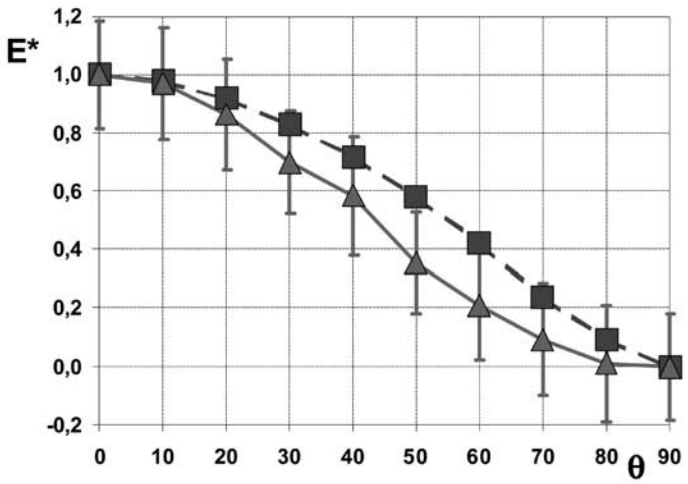

Fig. 1. The rescaled energy $E^*=U/U_{max}$ versus the tilt angle θ (in degrees) as obtained from Monte Carlo simulations (triangles) and by minimizing the elastic energy for the director configurations [13].

RESULTS

The dependence of the energy on the surface tilt angle θ is shown in *Fig. 1*. The MC results are compared with rescaled values obtained by means of an elastic continuum approach where the elastic energy was minimized for the director configuration inside the nematic spherical drop using a finite element technique [13].

The calculation of $\langle P_2 \rangle_\lambda$ in concentric shells starting from the center of droplet (shown in *Fig. 2)* for various values of the angle θ gives an indication of how the defect moves from the center of the droplet toward the surface. In fact, we can see that for perfect hedgehog configuration the maximum value of $\langle P_2 \rangle_\lambda$, corresponding to an aligned core which identify the defect at the inner shell, is very high (≈ 0.9) [14]. Increasing slightly the tilt angle we have a decreasing of the value of $\langle P_2 \rangle_\lambda$ at the first shell, because the configuration is still radial on average, but the defect moves toward the surface. As the tilt angle still increases the configuration becomes more and more bipolar and $\langle P_2 \rangle_\lambda$ at the center increases again.

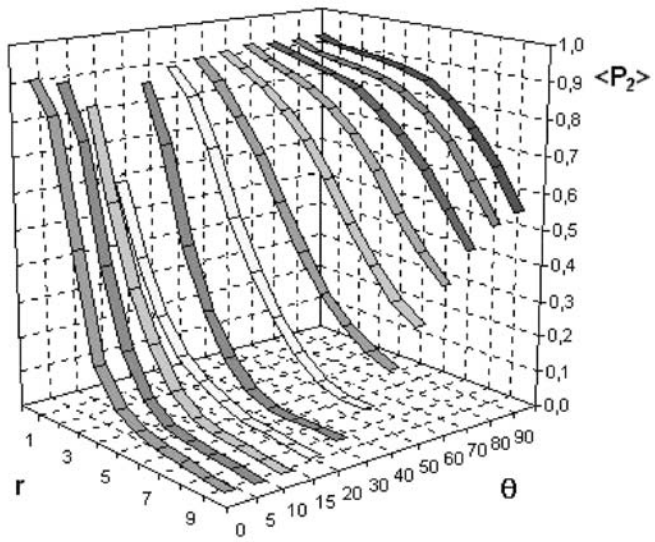

Fig. 2. The second rank order parameter dependence on the distance from the center of the droplet for various values of the anchoring tilt angle θ (in degrees).

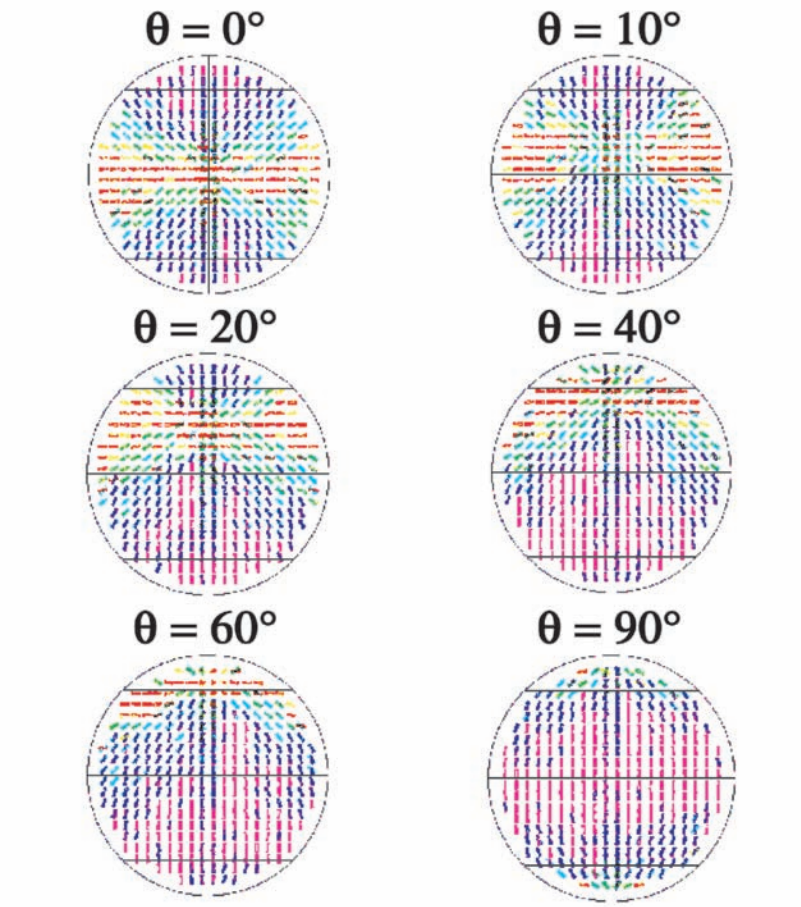

Fig. 3 Sample snapshots of the nematic droplet for some values of the tilt angle. The color code of the spins is chosen to help identifying the defect and depends on the angle between the spin orientation and the z axis. The discrete color palette is the following: magenta (along z), blue, cyano, green, yellow, red (perpendicular to z).

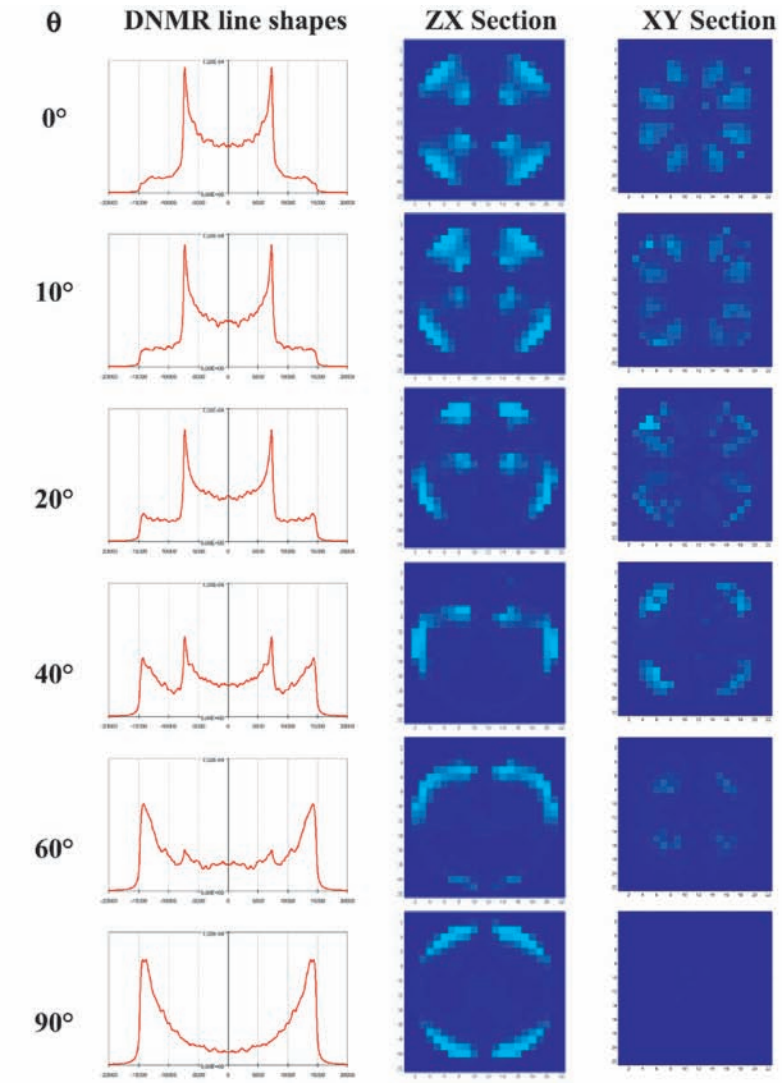

Fig. 4. Simulated experimental observables. DNMR spectra (left) and optical textures between crossed polarizers (right) for the nematic droplet for some values of the tilt angle (see text and ref. [6]).

The change in position of the defect is clear observing some sample snapshots reported in *Fig. 3*. As the tilt angle increases the point defect at the centre of the hedgehog configuration moves toward the pole of the droplet and splits in two boojums when a fully bipolar configuration is achieved. This is confirmed also by looking at the simulated experimental observables obtained from the Monte Carlo configurations as described in detail in Ref. [6]. These results are shown in Fig. 4.

CONCLUSIONS

We have performed Monte Carlo simulations of a nematic droplet with varying boundary conditions. Our simulations are based on the simplest lattice potential proposed to describe nematic liquid crystals, i.e. the Lebwohl-Lasher one. The calculation of the spin organization and of the ordering inside the droplet confirms the approaching of the point defect toward the droplet poles as the anchoring tilt angle varies and the boundary conditions become more and more bipolar.

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