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C. Chiccoli [a], P. Pasini [a], G. Skačej [b c] & C. Zannoni [c]

[a] Istituto Nazionale di Fisica Nucleare, Sezione di Bologna, Via Irnerio, Bologna, Italy

[b] University of Ljubljana, Physics Department, Jadranska, Slovenia

[c] Università di Bologna, Dipartimento di Chimica Fisica e Inorganica and INSTM, Viale Risorgimento, Bologna, Italy

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C. Chiccoli
P. Pasini
Istituto Nazionale di Fisica Nucleare, Sezione di Bologna, Via Irnerio, Bologna, Italy

G. Skačej
Istituto Nazionale di Fisica Nucleare, Sezione di Bologna, Via Irnerio, Bologna, Italy
University of Ljubljana, Physics Department, Jadranska, Slovenia
Università di Bologna, Dipartimento di Chimica Fisica e Inorganica and INSTM, Viale Risorgimento, Bologna, Italy

C. Zannoni
Università di Bologna, Dipartimento di Chimica Fisica e Inorganica and INSTM, Viale Risorgimento, Bologna, Italy

We present a Monte Carlo (MC) simulation of a nematic film with boundary conditions that vary from a homogeneous to a homeotropic anchoring at one surface while having a homogeneous anchoring at the other one. The simulations are based on the Lebwohl–Lasher lattice spin model with suitable boundary conditions to mimic the cell. We have investigated temperature effects on the molecular organization inside the system by calculating the internal energy, the heat capacity and the standard nematic order parameter.

Keywords: boundary conditions; liquid crystals; Monte Carlo; Nematic film

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Address correspondence to P. Pasini, INFN- Ser di Bowgna, Via Irnerio 46, Bologna, 40126 Italy. E-mail: pasini@bo.infn.it

INTRODUCTION

Nematic liquid crystals films continue to receive a great deal of attention, both for their applications in display technology and for their fundamental interest concerning the behaviour of mesophases in a restricted environment [1]. These systems consist of nematics placed between two suitably treated surfaces and the molecular organization in the liquid crystal can be strongly influenced by the boundary conditions. Even if the surface boundary conditions will tend to influence primarily the orientation of molecules near to the surface, the aligning effect may propagate inside the film. In general there will be a competition or anyway a combination of effects between the molecular orientation induced by the surface treatment, 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 set of boundary conditions will depend on a number of factors, including the strength of the surface interaction, the temperature and so on. We have shown in previous papers that, despite their simplicity, Monte Carlo simulations of lattice spin models can be a particularly effective tool to predict the combined effect of these factors in confined systems of various shapes [2]. Moreover, Monte Carlo simulations are also suitable to investigate the creation and the evolution of defects induced by the boundary conditions at the surfaces of nematic films [3,4]. From the ordering point of view a particular interesting case is the hybrid one where the anchoring is perpendicular to the surface (homeotropic) on one side and along a certain in-plane direction (homogeneous) on the other one. These opposite boundary conditions cause, for sufficiently thin films, a structural transition from the biaxial to the bent-director structure when the temperature of the system is lowered [5–7].

Here we wish to investigate, by computer simulations of a lattice spin model, a nematic film where the boundary conditions vary from a homogeneous configuration to a hybrid one. Such changes could in principle be obtained, e.g. by an appropriate illumination after covering the surface with a suitable photoresponsive material [8,9]. We shall see that, when changing the surface tilt angle from planar to homeotropic anchoring at the command surface, there is a change from a more stable nematic configuration to a configuration with a biaxial structure near the centre of the cell.

THE SIMULATION MODEL

The Monte Carlo simulations were based on the simple and well studied Lebwohl–Lasher (LL) spin model [10]. The particles interact

through the attractive nearest neighbours LL pair potential

$$U_{ij} = -\varepsilon_{ij} P_2(\cos\ \beta_{ij})$$

where

$$\varepsilon_{ij} = \begin{cases} \varepsilon & \varepsilon > 0 \quad \textit{for ij nearest neighbours} \\ 0 & \textit{otherwise} \end{cases}$$

β_{ij} is the angle between the axis of the two particles and P_2 is a second rank Legendre polynomial. The spins represent a cluster of neighbouring molecules whose short range order is assumed to be maintained through the temperature range examined [2]. The bulk Nematic-Isotropic (NI) transition temperature for this model occurs at $T^* = KT/\varepsilon = 1.232$ [11].

The different boundary conditions are mimicked assuming a layer of outside particles with a fixed orientation consistent with the desired type of alignment at the top and at the bottom surfaces. Periodic boundary conditions are employed at the four lateral surfaces of the simulated sample.

As we have mentioned before, in this work we have considered boundary conditions that vary from a homogeneous alignment to a homeotropic one at the top surface while at the bottom the alignment is considered to be always planar and homogeneous (along the x direction). To take into account this variation we have introduced the tilt angle θ between the spin orientation and the x axis at the top surface, then the angle θ ranges from $\theta = 0^\circ$ (planar homogeneous) to $\theta = 90^\circ$ (homeotropic).

To generate the lattice configurations we have used the standard Metropolis Monte Carlo procedure [12] where one spin at a time is updated as described in [2].

SIMULATION RESULTS

We have performed a set of independent complete simulations for a wide temperature range for various values of the surface tilt angle, i.e. $\theta = 0^\circ$, 5°, 10°, 15°, 30°, 45°, 60°, 70°, 80°, 85° and 90°. The simulated film is a $30 \times 30 \times (10 + 2)$ lattice. We calculate energy, $\langle U \rangle$, the second rank order parameter $\langle P_2 \rangle_\lambda$, as obtained from the largest eigenvalue of the ordering matrix, for the whole system and at each layer of the film [2,3]. We have also calculated the fourth rank order parameter $\langle P_4 \rangle_\lambda$ (not reported here for conciseness) and a nematic order parameter $\langle P_2 \rangle_x$ calculated with respect to a laboratory fixed direction, the x one.

In addition we have used the Monte Carlo configurations to directly simulate, by means of a simple matrix approach [2,13], optical microscopy images as could be obtained from the film between crossed polarizers. We describe each lattice site in the sample by a Müller matrix, so that the plane of polarization of a light beam travelling through a sequence of sites across the layers of the system will be rotated by the matrix resulting from the product of the Müller matrices corresponding to each encountered site. The light retarded by the spins in the film is then observed with the help of crossed polarisers 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 grey scale.

RESULTS

In Figure 1 we report the temperatures at which the peaks in the heat capacity occur as the tilt angle of the anchoring at the top surface changes from $\theta = 0^\circ$ (in plane) to $\theta = 90^\circ$ (homeotropic), while the other is kept at $\theta = 0^\circ$.

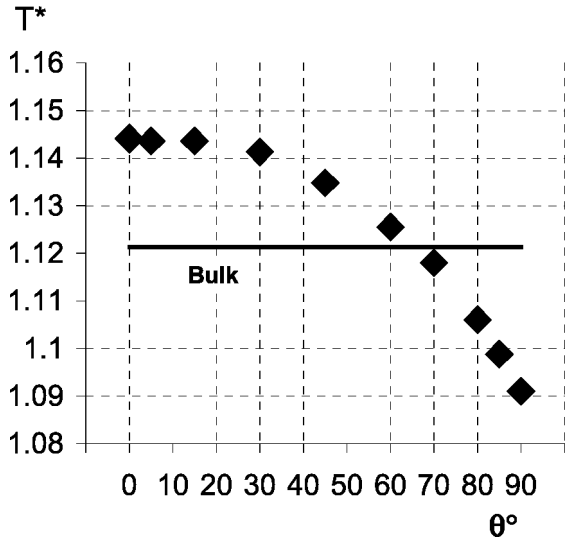

FIGURE 1 The heat capacity peak temperature for the various tilt angles θ (in degrees) asobtained from Monte Carlo simulations. The nematic-isotropic transition temperature for the LL model in the bulk is also reported (thick line).

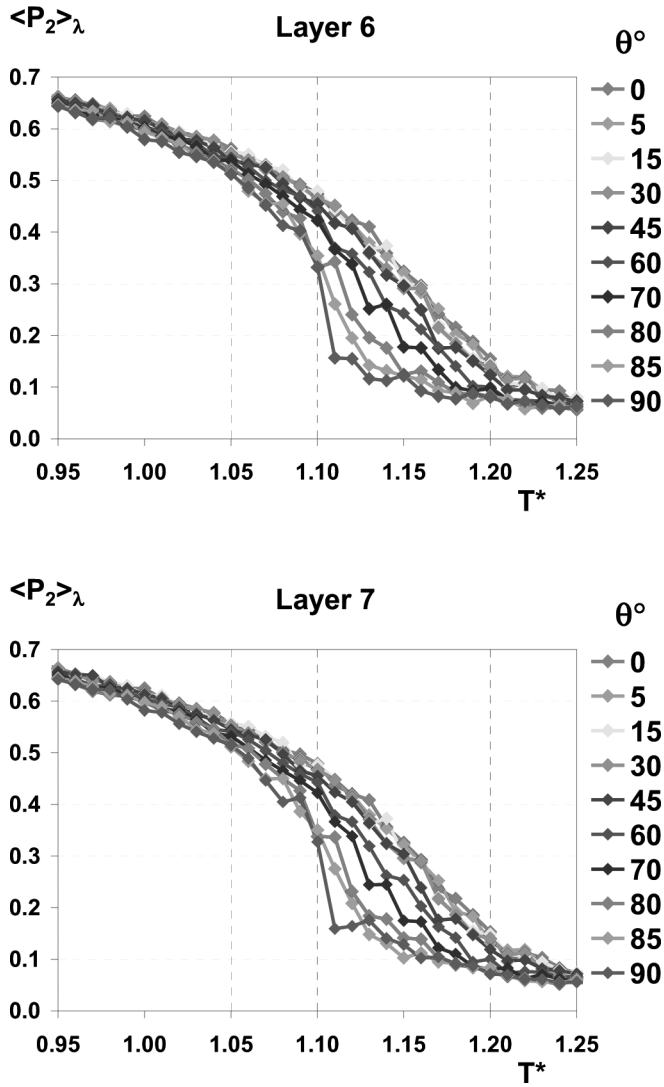

FIGURE 2 The second rank order parameter $\langle P_2 \rangle_\lambda$, calculated at the two central layers (6th and 7th) of the system, for various values of the anchoring tilt angle θ (in degrees). (See COLOR PLATE XXXII)

The curve indicates that, upon increasing the tilt, the peak position is stable around the homogeneous surface value $T^* \approx 1.145$ until the tilt angle approaches the value of 30° and then decreases. The overall

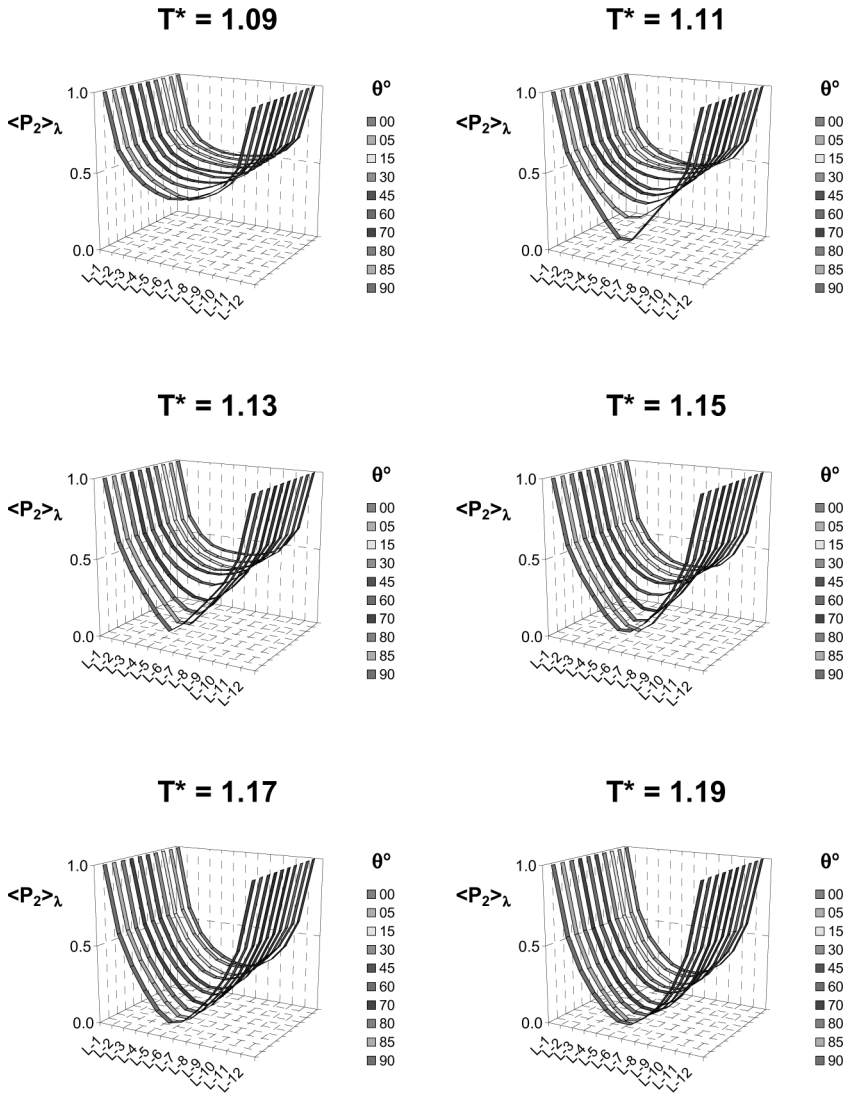

FIGURE 3 The second rank order parameter $\langle P_2 \rangle_i$, calculated at each layer of the system, starting from the bottom surface (L-1) of the film, for various values of the anchoring tilt angle θ (in degrees). (See COLOR PLATE XXXIII)

effect of changing the anchoring towards a homeotropic one on is then to shift the N-I transition to a lower temperature (up to $\approx 2.5\%$) with respect to the bulk one with a sharper decrease of the order parameter

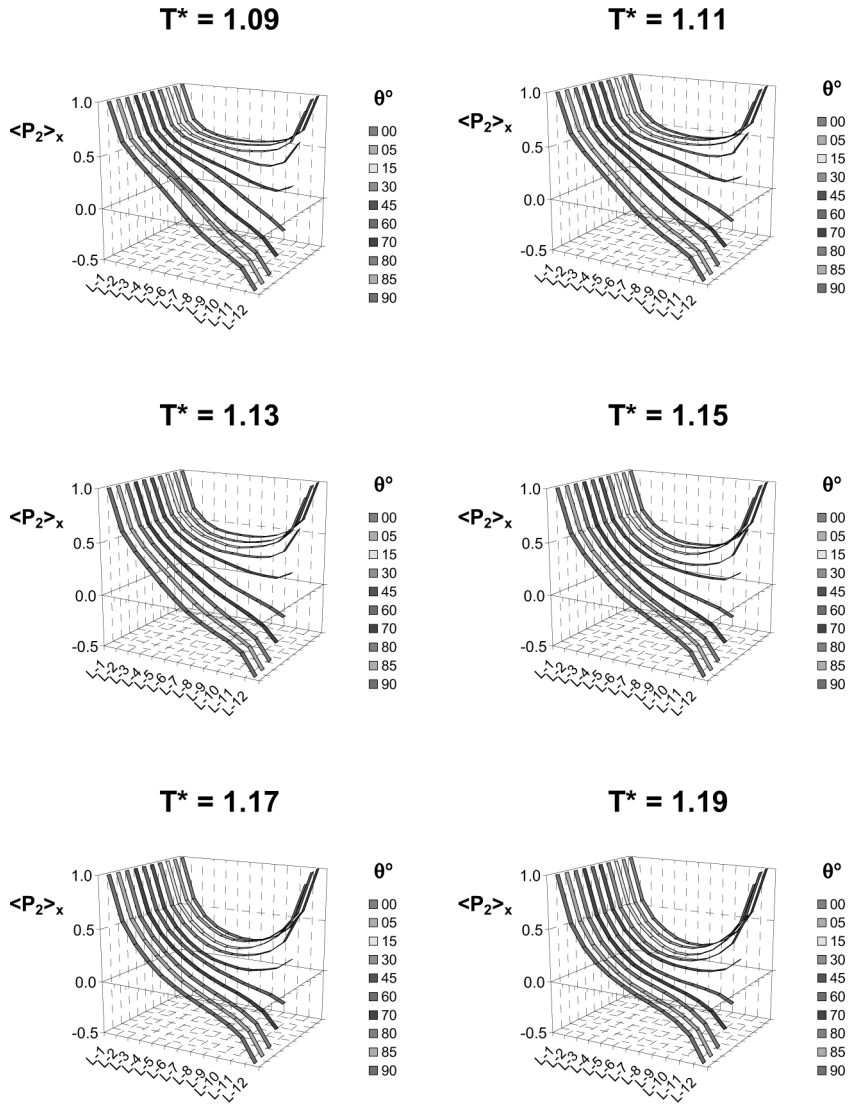

FIGURE 4 The second rank order parameter $\langle P_2 \rangle_x$ dependence on the distance from the bottom surface of the film for various values of the anchoring tilt angle θ (in degrees). (See COLOR PLATE XXXIV)

values across the transition. The order profile has been examined at each layer and the smoothing has been found to occur also at the center of the cell where the influence of the surfaces is lower (see Fig. 2). It is also interesting to notice that the main effect on the order occurs for

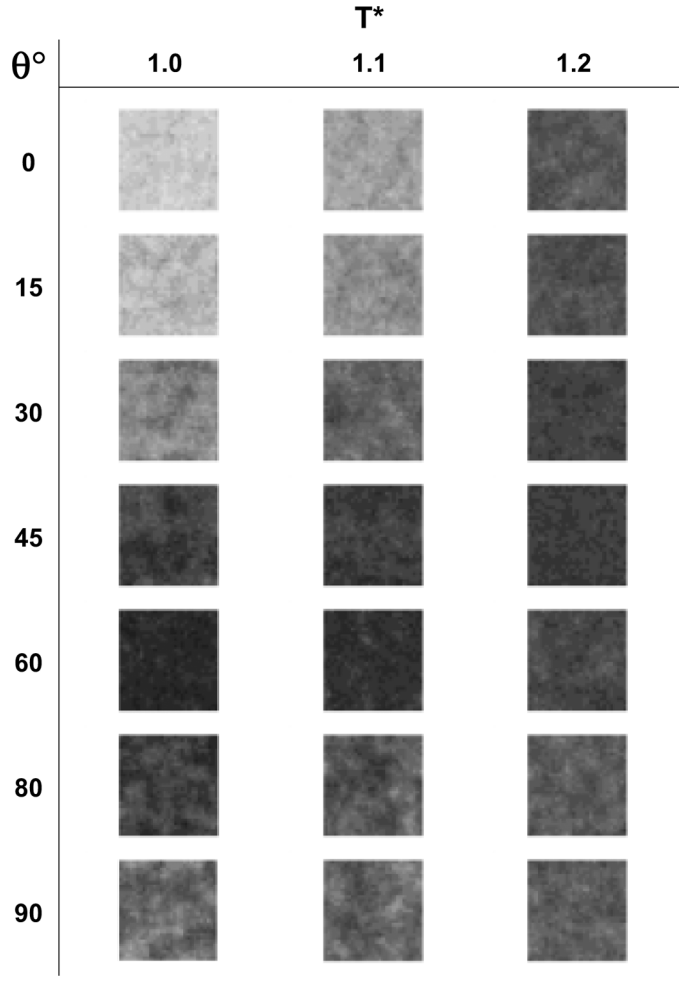

FIGURE 5 Simulated optical textures between crossed polarizers obtained for the nematic films with the reported values of the surface tilt angle θ.

high values of the tilt angle, i.e. when the surfaces have contrasting anchoring, at least for the film thickness here studied, and that the crossing with the bulk line is reached for $\theta \approx 70^{\circ}$.

This behaviour is also confirmed by examining the order parameters, $\langle P_2 \rangle_{\lambda}$ and $\langle P_2 \rangle_x$, calculated at each layer starting from the bottom of the film (L-1) and approaching the upper surface (L-12) for the various tilt angles considered (see Fig. 3 and Fig. 4). From the various curves plotted in a temperature range embracing the

transition, the different behaviour for the highest values of θ is apparent. The decrease in the ordering in the middle of the sample is very sharp in the case of hybrid alignment ($\theta = 90^\circ$) and becomes more and more continuous as the tilt angle decreases. The reason is that for the hybrid film of such thickness a bending transition still occurs from a biaxial to bent-director structure [7]. It seems that, since the thickness of the film is at the limiting value for the existence of such structural transition, a small variation from perfect hybrid boundaries is sufficient to move to a more stable molecular organisation.

The analysis of the optical textures confirms the considerations made by looking at the order parameters and at the heat capacity that just a small variation from the hybrid configuration rapidly leads to a molecular reorganisation inside the film. In Figure 5 we report these optical patterns for various values of the tilt angle for three selected temperatures in the neighbourhood of the transition. We can notice that for $\theta = 90^\circ$ we have an image compatible with a uniform configuration [3] at the lower temperature, configuration which becomes isotropic above the transition ($T^* = 1.2$). The pattern corresponding to a uniform configuration is less pronounced at $T^* = 1.0$ for $\theta = 80^\circ$ and completely lost for $\theta = 70^\circ$.

CONCLUSIONS

We have performed Monte Carlo simulations of a nematic film with varying boundary conditions. Our simulations are based on the simplest successful lattice potential put forward to describe nematic liquid crystals, i.e. the Lebwohl–Lasher one. Our results are consistent with a rapid change from a uniform configuration, with a structural transition in the centre of the sample, for the hybrid film to a more ordered and stable molecular organisation as the tilt angle taking with respect to the upper surface decreases. The results are obtained for a film thickness for which the structural transition is still present even though it is more evident in thinner films.

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