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Cesare Chiccoli [a] , Paolo Pasini [a] , Ivan Feruli [b] & Claudio Zannoni [b]
[a] INFN, Sezione di Bologna, Via Irnerio 46, 40126, Bologna, Italy
[b] Dipartimento di Chimica Fisica ed Inorganica and INSTM-CRIMSON, Viale Risorgimento 4, 40136, Bologna, Italy
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Computer Simulations of Inversion Walls in Nematic Films

CESARE CHICCOLI,[1] PAOLO PASINI,[1,*] IVAN FERULI,[2] AND CLAUDIO ZANNONI[2]

[1]INFN, Sezione di Bologna, Via Irnerio 46, 40126 Bologna, Italy
[2]Dipartimento di Chimica Fisica ed Inorganica and INSTM-CRIMSON, Viale Risorgimento 4, 40136 Bologna, Italy

Monte Carlo simulations of lattice spin models are employed to investigate the creation of inversion walls in nematic films with specific boundary conditions. The simulations, based on the well known Lebwohl-Lasher potential, allow to produce simulated polarized microscopy images which are followed during their evolution and analysed for different film thicknesses.

Keywords Computer simulation; Monte Carlo; nematic liquid crystals; topological defects

Introduction

A very important aspect of liquid crystal (LC) materials is that they exhibit various classes of topological defects [1,2], offering the possibility of a convenient laboratory for the experimental study of these singularities. The study of topological defects in liquid crystals [1,2] has indeed proved to be of great importance from a number of stand points ranging from mathematics [1,3] to theoretical physics [4–7], cosmology [9,10] and nano-technology [11,12]. Defects in LC can be operationally defined as regions (points, lines, walls . . .) where the director field presents a discontinuity of some kind and the scalar order parameter goes to zero.

The theoretical investigation of defects and their structure is typically performed by setting up a Frank elastic constant free energy F for a liquid crystal, endowed with certain elastic constants, confined to a given geometry and subject to prescribed anchoring conditions and then searching for director fields that minimize F. Given the difficulty of achieving analytic solutions, a numerical approach is often followed and simulated structures are obtained [13–17]. In a relatively small number of cases [6–8,18] an opposite, bottom up approach to the director field structure has instead been followed, starting from a microscopic, molecular level, Hamiltonian and performing a statistical mechanics, typically Monte Carlo [19] simulation. This approach has some advantages, in that it does not require explicit input of material constants but just of a pair potential and that it creates a direct link between microscopic and macroscopic properties.

*Address correspondence to Paolo Pasini, INFN, Sezione di Bologna, Via Irnerio 46, 40126 Bologna, Italy. E-mail: pasini@bo.infn.it

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In the present paper we aim to investigate the creation and evolution of a particular type of defects, the inversion walls, i.e. two dimensional regions where the director is not defined. Inversion walls are typically created following the relaxation of an homogeneous sample in a suitable geometry where the transient appearance of the defect can be stabilized. There are various types of defect walls, e.g. splay-bend, bend-splay and twist walls [1,2,20]. In particular the liquid crystal can be subject to twist deformations, corresponding to rotations around a defined and unique axis, which can be identified in the sample. In a region where the twist is uniform the director remains orthogonal to the rotation axis describing a helix around it. However, being the nematics formed by non-polar and non-chiral molecules there is no preferred sense for the helix twist, as both the two directions for rotating around the axis have the same probability. An inversion wall is thus generated at each boundary between domains with opposite twist.

Here we present the simulation of inversion walls obtained by imposing conical tangential boundary conditions at the top and bottom surfaces of the thin film sample. In this case the easy axis, i.e. the direction along which the molecules tend to align, at the surfaces is distributed on a cone. We follow the relaxation of the system from an initially homogeneously aligned sample using Monte Carlo method and we describe the characteristic of the wall obtained and its behavior in an external field.

The Simulation Model

We use the Lebwohl-Lasher (LL) lattice model well studied in detail by computer simulations of bulk systems [21,22] and also of confined samples [23]. In the bulk it reproduces the orientational properties and the characteristics of the nematic isotropic phase transition. The model hamiltonian is the following:

$$U_N = (1/2) \sum_{\substack{i,j \in F \\ i \neq j}} \Phi_{ij} + J \sum_{\substack{i \in F \\ j \in S}} \Phi_{ij} \tag{1}$$

where F, S are the set of particles in the bulk and at the surfaces, respectively, and the parameter J models the strength of the coupling with the surfaces. The molecules, represented by three dimensional unit vectors $\boldsymbol{u}_i$ ("spins"), have cylindrical symmetry and tend to align their major axis due to the second rank attractive pair potential:

$$\Phi_{ij} = -\varepsilon_{ij} \, P_2(\cos \, \beta_{ij}) \tag{2}$$

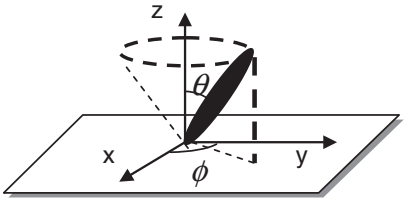

Figure 1. A sketch showing the molecular long axis at the boundary layer and the angles θ and ϕ.

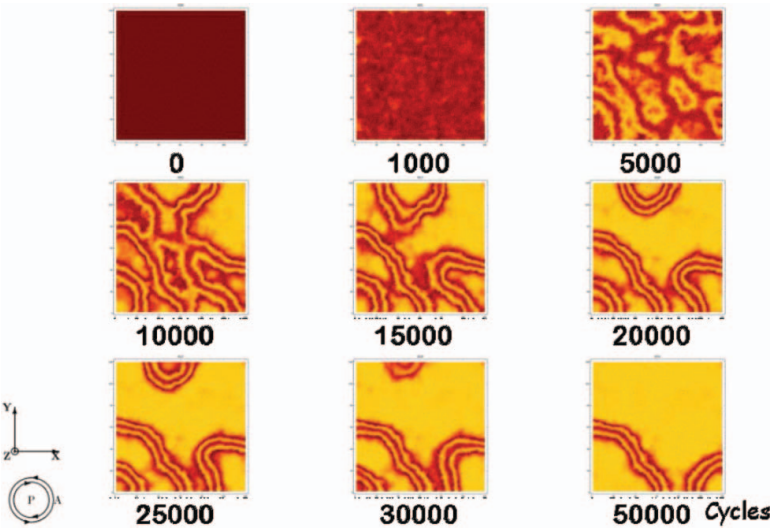

Figure 2. Evolution of optical textures as obtained from the simulation of a 120 × 120 × (8 + 2) nematic film. The images are simulated considering the film between left and right circular polarizers and are taken as the run progresses, at (0, 1, 5, 10, 15, 20, 25, 30 and 50 evolution kcycles).

where ε_{ij} is a positive constant, ε, for nearest neighbour molecules i and j and zero otherwise, β_{ij} is the angle between the axis of the two interacting spins and P_2 is the second Legendre polynomial [24].

While in simulating bulk systems periodic boundary conditions are employed, in the case of confinement the required boundaries are implemented by considering additional

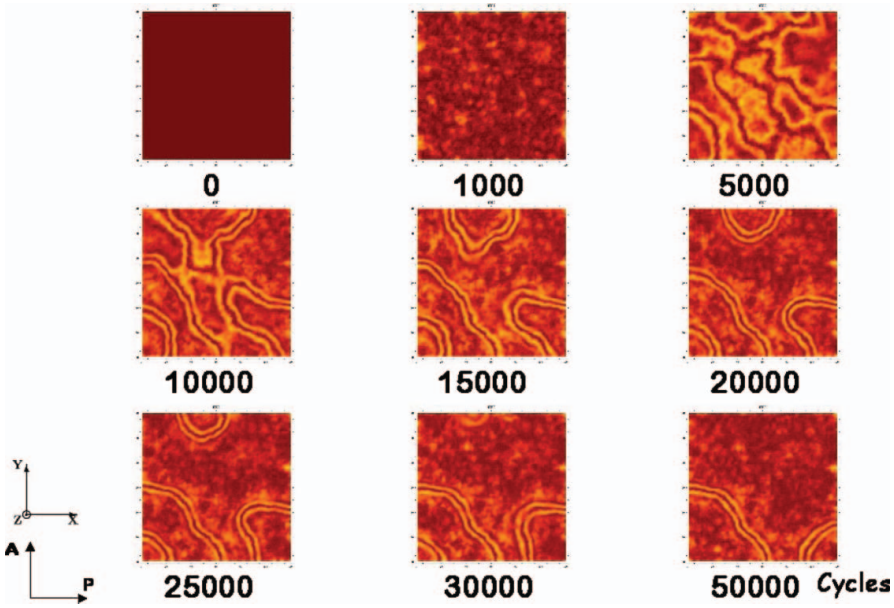

Figure 3. The same case as in Fig. 1 but as seen through crossed linear polarizers.

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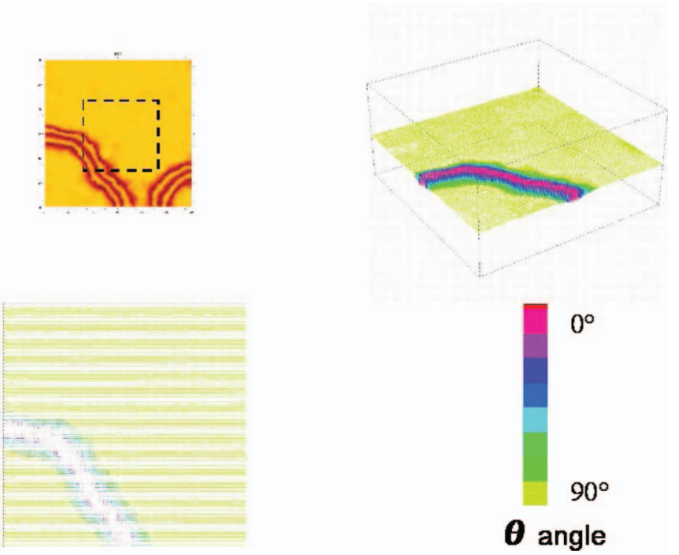

Figure 4. Snapshots of the central layer of the film corresponding to the portion of a 120 × 120 × (8 + 2) system enclosed by the dashed line square in the optical image. The color code indicates the value of the angle θ between the molecular axis and the z direction. This angle can vary from 0° (perfect alignment along z, red color) to 90° (molecule lying in the xy plane, green color).

layers of particles, kept fixed during the simulation, with suitable orientations chosen to mimic the desired surface alignment. We have studied uniaxial nematic droplets with radial, bipolar and toroidal boundary [23] and films with hybrid [8] and Schlieren geometries [25].

Here we present a detailed study of uniaxial nematic films with conical boundary conditions at the bottom and top surfaces of the simulation sample. The cone angle θ is chosen to be $\pi/4$, while the angle ϕ, between the projection of the long axis of the molecule

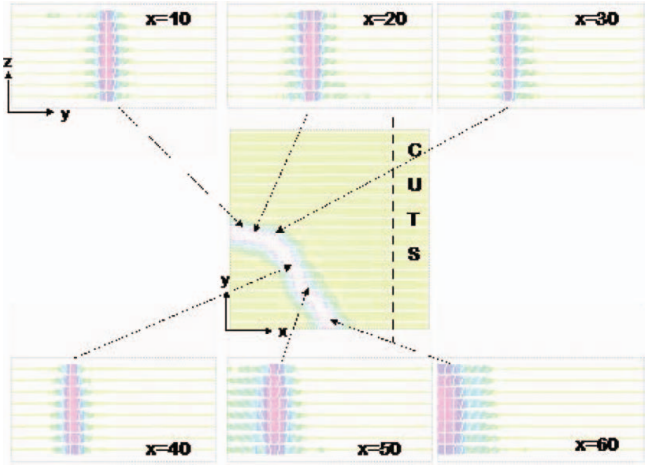

Figure 5. Vertical sections taken at various distance along the x axis of the lattice in the domain wall region. The color coding is the same as in Fig. 4.

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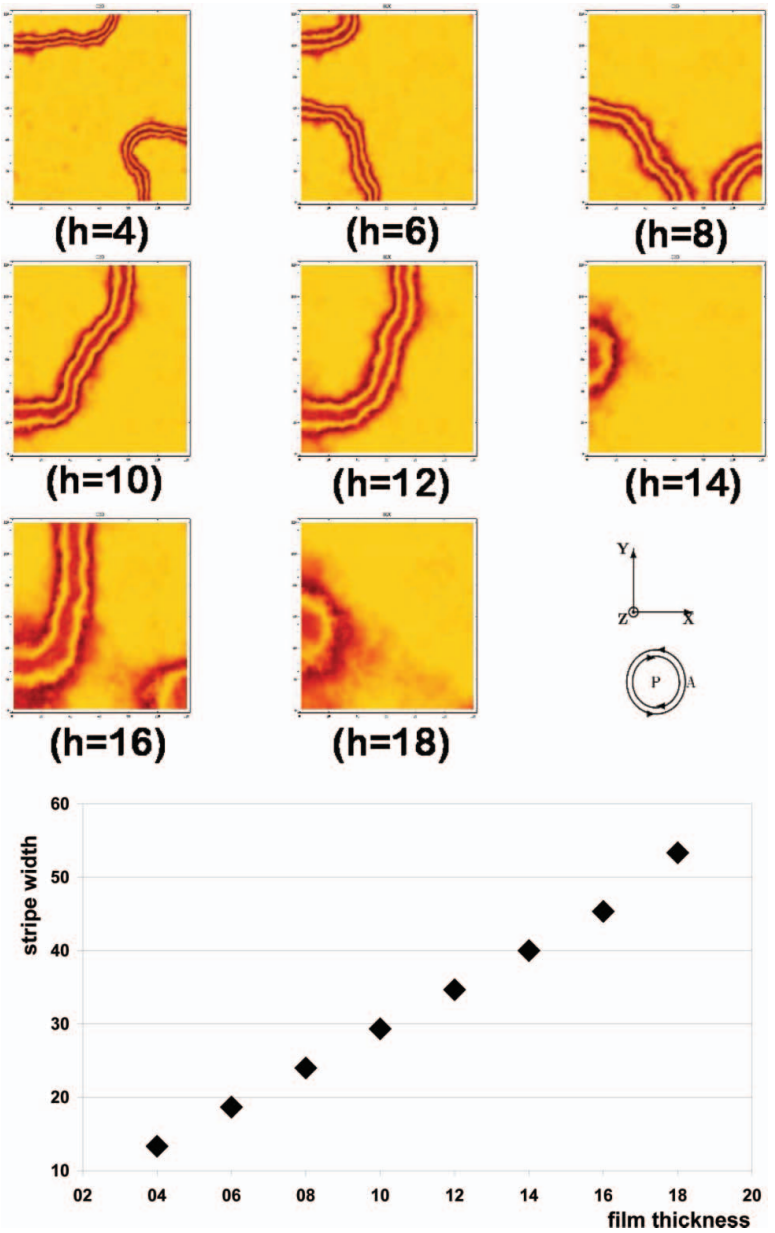

Figure 6. Simulated polarized optical images after 50000 MC cycles (top) and dependence of the stripe width (bottom) on the film thickness.

onto the *xy* plane and the *x* axis, is random (Fig. 1). At the four lateral faces of the system we employ free boundary conditions.

We have simulated systems of size $N = 120 \times 120 \times (h + 2)$ with the film thickness $h = 4,6,8,10,12,14,16,18$. The starting configurations of the lattice were chosen to be completely aligned along the z direction and the evolution of the system was followed according to the classic Metropolis Monte Carlo procedure [19] at the reduced temperature $T^* = kT/\varepsilon = 0.1$.

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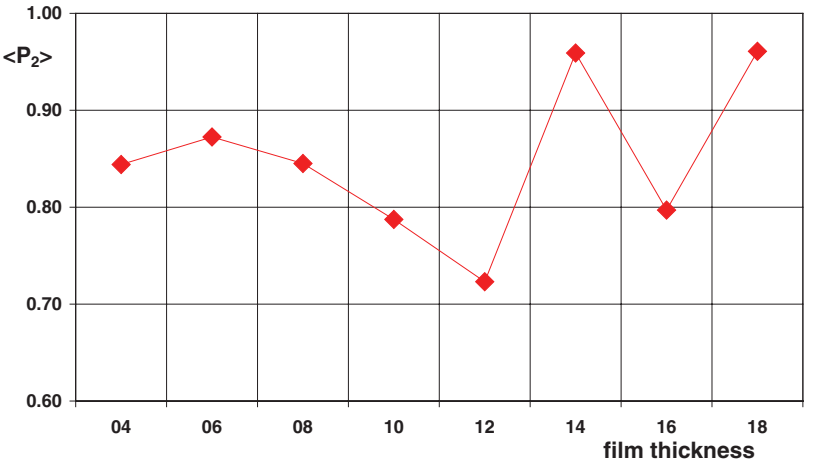

Figure 7. Second rank order parameter $<P_2>$ of the whole systems versus film thickness.

Polarizing microscope textures were simulated by means of a Müller matrix approach [23], assuming the molecular domains represented by the spins to act as retarders on the light propagating through the sample. The images are taken averaging over *1000* Monte Carlo cycles where a cycle is a complete attempt to update the lattice, i.e. N attempted moves. The optical parameters adopted are the following: film thickness $h = 5.3\ \mu m$, light wavelength $\lambda_0 = 545\ nm$ and ordinary and extraordinary refractive indices $n_o = 1.5$, $n_e = 1.66$.

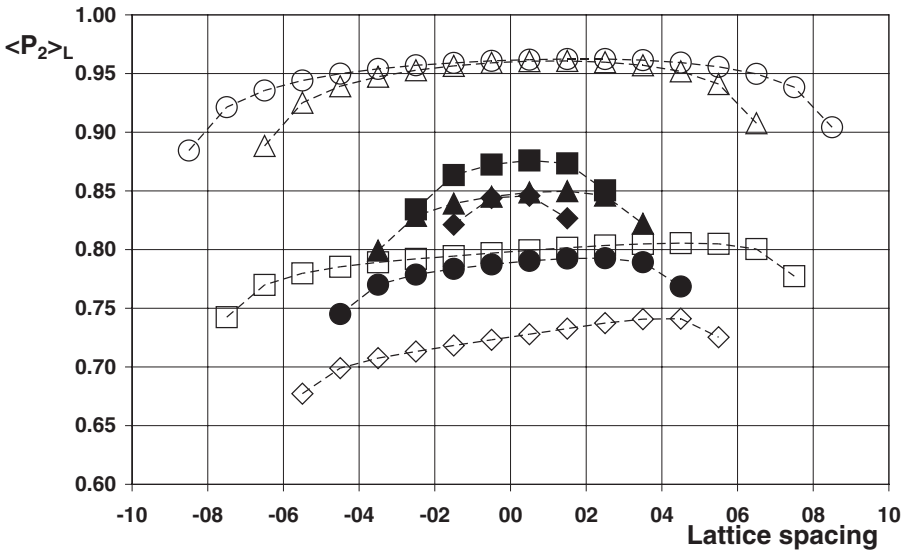

Figure 8. Nematic order parameter $<P_2>_L$ with respect to the z direction calculated for each layer of the systems starting from the center of the lattice. The symbols correspond to the following film thicknesses: h = 4 (full diamond), h = 6 (full square), h = 8 (full triangle), h = 10 (full circle, h = 12 (empty diamond), h = 14 (empty triangle), h = 16 (empty square), h = 18 (empty circle).

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Simulations and Results

A set of independent simulations have been performed for different film thickness at a temperature deep in the nematic phase ($T^* = 0.1$). In Figs. 2 and 3 we report a typical evolution of the optical textures observed for a $120 \times 120 \times (8 + 2)$ system at various Monte Carlo cycles as obtained by simulating circular (Fig. 2) and crossed linear (Fig. 3) polarizers. It can be noticed that after some thousands cycles a network of defects appears which evolves in domain walls. The molecules of the thin film tend to lie on the *xy* plane apart from those responsible of the creation of the domain wall.

In this case the molecules, especially those belonging to the central layer are aligned along z as can be seen from Fig. 4 and Fig. 5.

Their nearest neighbours tend to recover the alignment orthogonal to the z direction. In the stripe the light intensity varies through maxima and minima. This variation is clear by looking at the snapshots where it is evident that the angle θ formed by the molecular axis with the z axis has two rotation directions. The angle varies from 0 to $\pi/2$ and from 0 to $-\pi/2$ and this is the cause of the variation of the birefringence detected by the circular polarizers in the stripes. In fact, for uniaxial liquid crystals the birefringence depends only on the relative orientation between the local optical axis and the light propagation direction.

The width of the domain wall is an important feature of these defects [2]. In our simulations it corresponds to the average number of molecules that are aligned vertically. This number depends (approximately linearly) on the thickness of the film as can be seen in Fig. 6. These qualitative observations can be made quantitative by calculating the second rank order parameter for the whole system and for each layer of the films. We report in Fig. 7 the nematic order parameter calculated for each film thickness on the whole system after 50000 Monte Carlo Cycles. It is evident that increasing the thickness of the film the order parameter decreases as the width of the domain wall increases. This is true for the thinner films because when the thickness is larger, at least in our simulations, the domain wall can move outside the sample. In Fig. 8 we show the nematic order parameter with respect to the z direction calculated at each layer of the systems.

Conclusions

We have verified the appearance of inversion walls in nematic uniaxial films when the anchoring direction of the molecules at the surfaces is tilted and tends, on average, to be distributed on a cone and we have described them at microscopic level. After the Monte Carlo equilibration runs the cells appear divided in two regions where the orientations of the molecules are uniform. The two blocks are separated by a stripe region where the intensity of the transmitted light varies between maxima and minima, as it is evident looking at the snapshots of the middle layer. The width and the persistence of the domain walls depend on the film thickness, i.e. increasing the thickness the stripe width increases. We have shown in previous works that a larger thickness gives a behaviour similar of a thinner film where the coupling/anchoring of the molecules at the surfaces is weaker.

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