International Journal of Modern Physics C, Vol. 6, No. 1 (1995) 135-141

A MONTE CARLO SIMULATION OF A TWISTED NEMATIC LIQUID CRYSTAL DISPLAY

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Received 25 September 1994

We present a Monte Carlo simulation of a model of a twisted nematic display on a lattice starting from purely microscopic interactions. We visualize the simulated display calculating optical textures under crossed polarizers corresponding to the Monte Carlo microscopic configurations. We also investigate the orientational order and the molecular organizations in the different regions of the lattice, introducing and calculating suitable order parameters.

Keywords: Liquid Crystal Display; Computer Simulations.

1. Introduction

Liquid Crystal Displays (LCDs), especially of the "twisted nematic" type,[1] are commonly used since the early 70s and are now one of the electro-optical devices most often used in the world. While a large part of the know-how on LCDs seems to be empirical or based on macroscopical models, the range and scale of computer modeling have now grown to the point where it is possible to try and attempt a complete simulation of a model display starting from microscopic interactions. We have therefore elaborated a simple spin model using Monte Carlo (MC) simulations both to demonstrate the feasibility of this approach and as a tool to investigate the molecular organization within a LCD system. The MC method has already proved to be a powerful tool for microscopic understanding of liquid crystal models, as can be seen from the steadily increasing amount of work (see, e.g., Refs. 2–14) performed since the pioneering paper of Lebwohl and Lasher.[2] In particular, we have shown that MC simulations can be especially useful for investigating the effect of various individual and combined factors, such as boundary conditions, anchoring strength, temperature and external applied fields,[8,12–14] on the molecular organization of confined nematic systems such as PDLCs (Polymer Dispersed Liquid Crystals).[15,16] In the presence of impurities, inhomogenities and, in general of conditions that

constitute prohibitive difficulties for analytical theories, we believe that MC can provide a unique tool for understanding and predicting ordering and microscopic organization.

This work was started as an attempt to test if our simple models can be used to simulate a twisted nematic LCD. In what follows, we shall briefly describe the model employed and the visualization technique and show the results obtained both at macroscopic and microscopic level.

2. Monte Carlo Simulations

Just as for a real display, we need a nematic between two aligned surfaces. Here we have chosen a Lebwohl–Lasher (LL) nematic which consists of a system of "spins" placed on a cubic lattice and interacting through the second rank potential[2]:

$$U_{ij} = -\epsilon_{ij} P_2(\cos\beta_{ij}) \tag{1}$$

where ϵ_{ij} is a positive constant for nearest neighbors particles i and j and zero otherwise, β_{ij} is the angle between the axes of the two molecules, and P_2 is a second rank Legendre polynomial.

The model, although very simple, gives a good representation of the orientational properties of a real nematic, (i) showing a weak first order phase transition to an isotropic state (at a scaled temperature $T^*_{NI} \equiv kT_{NI}/\epsilon = 1.1232$), (ii) including a reasonable dependence of the orientational order parameter $\langle P_2 \rangle$ on temperature and even (iii) pretransitional effects diverging, like for real nematics, just below T^*_{NI}.

We suggest that the model works so well because a "spin" represents a closely packed group of molecules, rather than a single particle, and that this micro-domain maintains its local structure at various temperatures and even across the nematic–isotropic phase transition.[17] As a special case, these domains could comprise just one molecule but it seems realistic to assume that they could include a few tenths of particles.[13,14]

The simplicity of the LL model allows the performance of simulations on a relatively large number of spins in comparison to models assuming "more realistic" potentials with translational degrees of freedom. In the present calculations, we include up to about 30000 spins in a cell. As already mentioned, our display model is constructed on a lattice, and we have considered a system with boundary conditions that mimick the orthogonally aligned cell surfaces placing a layer of fixed aligned spins at the top and at the bottom of the lattice (see Fig. 1). Periodic boundary conditions are employed around the other four faces of the cube. Moreover, the lattice is divided into a regular array of sublattices where a field can be applied. At a microscopic level, this is realized adding another second rank term to the LL Hamiltonian[3,12]:

$$U_N = -\sum_{\substack{i \neq j \\ i<j}}^{N} \epsilon_{ij} P_2(\cos\beta_{ij}) - J\epsilon\xi \sum_{i=0}^{N} P_2(\cos\beta_i)\,. \tag{2}$$

Here β_i is the angle between the field direction and the spin axis, ξ determines the strength of coupling to the field $\mathbf{B}$ (directed along the z axis), while the parameter $J = 1$ or 0 acts as a switch to turn on or off the local external field. We assume that an electric field is applied and we take $\xi > 0$, corresponding to a material with positive dielectric anisotropy. In the absence of the field (*off* region) the effect of the orthogonally oriented boundary conditions tends to propagate inside the system producing a twisted nematic configuration. On the contrary, when a sufficient strong field is applied (*on* region), the molecules on which it acts change their orientations on average aligning themselves along the field direction as schematically shown in Fig. 1.[1]

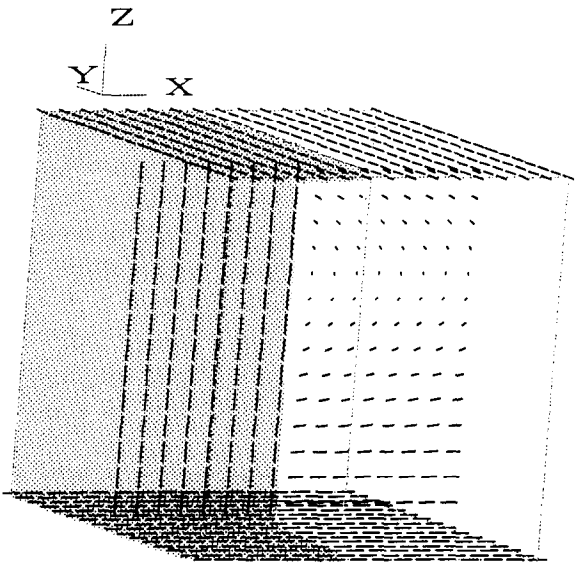

Fig. 1. The orthogonally aligned surfaces at the top and at the bottom of the lattice, together with a subset of spins in the regions where the field is *off* and *on* (grey area).

The standard Metropolis Monte Carlo procedure described in our previous studies[7,8,11–14] has been used to update the lattice. We have used at least 150000 equilibration cycles before starting to accumulate the averages of the quantities of interest. Production runs were up to 50 kcycles. During the production run various observables, in addition to the internal energy and second rank order parameters, were calculated. Each property of interest, A, is evaluated at every cycle.

3. Visualization

To obtain an image from a simulated LCD configuration, we associate each site i in the display to a Müller matrix $\mathbf{M}_i$ using the standard approach which has been employed in calculations based on continuum theory[18,19] and in our earlier calculations of optical textures based on the configurations obtained from MC simluations

of PDLC.[13,14] The light beam traveling through a row of sites across the layers of the display is then retarded by the matrix resulting from the product of the Müller matrices $\mathbf{M}_i$ corresponding to each of these sites. The light modulated by the LCD is observed with the help of crossed polarizers placed on each side of the cell, $\mathbf{P}_{\text{in}}$ and $\mathbf{P}_{\text{out}}$. The Stokes vector[19,20] representing the retarded and polarized light $\mathbf{s}$ is then obtained by

$$\mathbf{s} = \mathbf{P}_{\text{out}} \prod_i \mathbf{M}_i \mathbf{P}_{\text{in}} \mathbf{s}_{\text{in}} \tag{3}$$

where $\mathbf{s}_{\text{in}}$ is the vector corresponding to unpolarized light. The crossed polarizers cut off the unretarded light, where the molecules are aligned along the applied field (*on* region), while the largest intensity of light goes through the polarizers for a perfect twist ordering (*off* region at low temperature). In our calculations, we have used refraction parameters similar to those of the nematic liquid crystal 5CB.[16] To improve the signal to noise ratio of the optical image, we have averaged over at least 20000 configurations sampled every 2 cycles.

In Fig. 2 we show the resulting visualized image of a simulated display at scaled temperature $T^* = 1.0$ and with an applied field strength $\xi = 1.0$ in the *on* regions. This value of ξ is probably too large to be realistic for current displays but is suitable for the present demonstration purposes. Each pixel of the display corresponds to a lattice point in the xy plane. The dimension of a layer is 30×50 and the image in Fig. 2 is made from a sample with ten layers inside the cell.

We have performed a set of independent simulations for various field strengths at different selected temperatures. The contrast of the grey scales in the optical

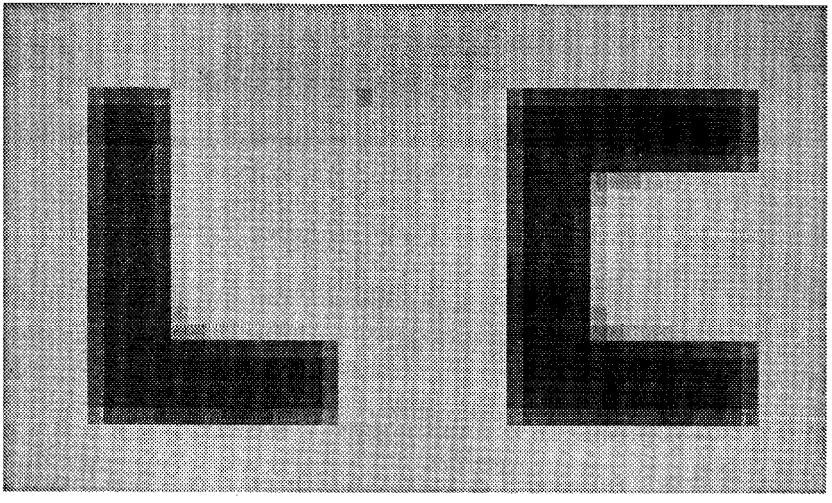

Fig. 2. Examples of display images as obtained from Monte Carlo simulations on a $50 \times 30 \times 10$ lattice. The applied field in the *on* regions has a strength of $\xi = 1.0$ and the reduced temperature, $T^* = 1.0$.

representation is, as expected, favoured by a large applied field and low temperature. However, we have chosen to present an image of a display at $T^* = 1.0$ that should roughly correspond to a room temperature nematic at reduced temperature $T/T_{NI} \approx 0.89$. To understand the effect of display thickness, we have investigated the dependence on the system size in the z direction, assumed to be parallel to the applied field, from ten to thirty layers, and have found the resolution of the optical texture to be already good for ten layers and then not to change much or to worsen. A comparison of the size dependence with that observed for specific real nematics could provide a way of establishing a correspondence between simulated and real cells.

4. Order Parameters

We have calculated, apart from the usual thermodynamic observables, some order parameters appropriate for determining the ordering in certain zones of the lattice,

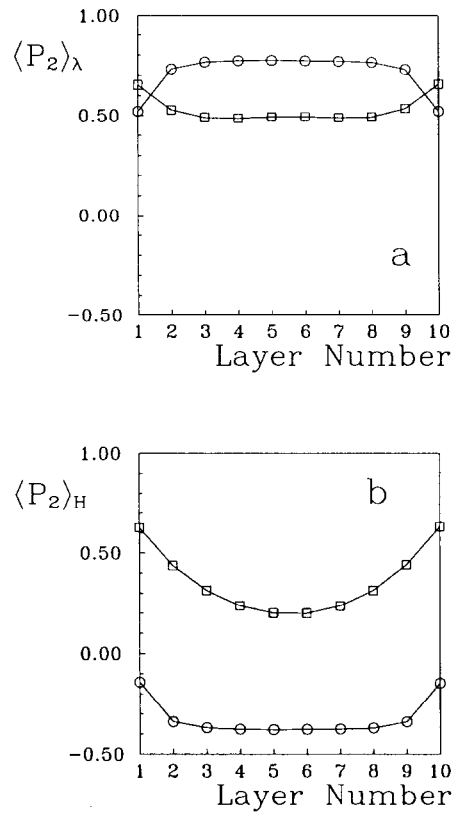

Fig. 3(a) The nematic order parameter $\langle P_2 \rangle_\lambda$ and (b) the helical order parameter $\langle P_2 \rangle_H$ across the display, in lattice units, in the two regions *on* (○) and *off* (□). The example reported is for the same simulation as presented in Fig. 2.

in particular, the different layers and in the two regions — those with external field *off* or *on*. The first quantity we have looked at is the standard order parameter $\langle P_2 \rangle_\lambda$, obtained from the largest eigenvalue of the ordering matrix,[2] which quantifies the nematic ordering. We have calculated $\langle P_2 \rangle_\lambda$ over all the system in the *on* and *off* regions and also on each layer to investigate how the oriented boundary conditions influence the liquid crystal inside the lattice (Fig. 3(a)). We see that $\langle P_2 \rangle_\lambda$ is, except near the surface, higher in the *on* than in the *off* region. Moreover, we have calculated, for each layer, a new kind of microscopic quantity that we call *helical order parameter*, $\langle P_2 \rangle_{\mathrm{H}}$ defined as follows:

$$\langle P_2 \rangle_{\mathrm{H}} = \frac{1}{N_L} \sum_{i=1}^{N_L} P_2(\mathbf{u}_i \cdot \mathbf{t}_i)\,, \tag{4}$$

where N_L is the number of particles contained in the Lth layer, $\mathbf{u}_i$ is the orientation vector for the ith spin and $\mathbf{t}_i$ is the ideal twist direction at point i. This parameter expresses disordering from a perfectly twisted organization, and $\langle P_2 \rangle_{\mathrm{H}} = 1$, when all the particles lie in the direction defined by the discretized helix between the bottom and top surfaces. For the perfectly twisted organization, we obtain the largest intensity of light through the display. The helical order parameter is plotted for each layer in Fig. 3(b). We see that $\langle P_2 \rangle_{\mathrm{H}}$ is always higher in the field *off* regions, even though it decreases moving from the surface to the centre of the cell. In the field *on* regions, $\langle P_2 \rangle_{\mathrm{H}}$ is negative corresponding to the molecules on average being perpendicular to the ideal helix axis.

5. Conclusions

We have, for the first time, simulated a twisted nematic display using a simple spin model, and presented the visualized result of the macroscopic image resulting from the MC simulation. We also present microscopic order parameters, describing the molecular ordering in different regions of the display, with and without an applied electric field. We believe the method introduced here can be applied to treat a variety of liquid crystal displays in a way that directly bridges the gap between microscopic interactions and observed macroscopic behavior.

Acknowledgments

We are grateful to MURST and CNR for support. E.B. thanks the Swedish NFR and EEC HCM.

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