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Computer Simulations of Nematic Displays

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Monte Carlo simulations of electroptical devices based on a nematic Lebwohl-Lasher liquid crystal model with suitable boundary conditions are presented. The simplicity of the model allows an investigation of various effects like the influence of an external field strength and that of anchoring at the oriented surfaces of the display cell. Moreover suitable order parameters are introduce to facilitate an understanding of the molecular organisation inside the electroptical cells.

Keywords: Monte Carlo; Twisted nematic display; In-plane switching effect

INTRODUCTION

Monte Carlo simulations have proved to be very useful in investigating liquid crystalline systems both in the bulk and in confined geometries [1]. The case of finite environments is a particular interesting one, even if simulations are more usually performed to investigate the physics of bulk systems. Confined liquid crystals have found their main technological application in displays, where the electroptical effects are based on some sort of light modulation due to the anisotropic material. Research and development of such devices have been carried out until now using empirical macroscopic models developed more than two decades ago [2]. We think that computer simulations, thanks also to the continuous increase in computing power, can now represent a useful tool to study the physics of displays starting from microscopic interactions. Recently

we have performed Monte Carlo simulations of Twisted nematic [2] and In-Plane Switching [3] displays by using a simple lattice spin model [4,5]. Here we briefly summarize the method and present some new results for the In-Plane Switching display.

THE SIMULATION MODEL

The simulation model is based on a Lebwohl - Lasher (LL) lattice spin system [6,7], where the molecules, assumed to be three dimensional "headless spins", are placed on the sites of a cubic lattice and interact through the second rank LL potential [6]:

$$U = -\sum_{i,j \in \mathcal{N}} \epsilon_{ij} \left[P_2(\mathbf{s}_i \cdot \mathbf{s}_j) \right] \tag{1}$$

where ϵ_{ij} is a positive constant, ϵ, for nearest neighbors 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. The spin $\mathbf{s}_i$ represents a cluster of neigboring molecules whose short range order is maintained through the temperature range examined [8].

The aligned surfaces of the display are simulated by imposing a fixed orientation to the spins belonging to the layers at the top and at the bottom of the cell [4,5]. Periodic boundary conditions are instead employed around the other four faces of the simulation box to reduce the size effects.

The application of an external field is implemented, at the microscopic level, by adding another second rank term to the LL hamiltonian [9,10] of molecule i:

$$U_{field}(\beta_i) = -J\epsilon\xi P_2(\cos\beta_i) \tag{2}$$

Here β_i is the angle between the field direction and the particle symmetry axis, the dimensionless constant ξ determines the sign and strength of coupling with the field $\mathbf{E}$ while the parameter $J = 1$ or 0 acts as a switch to turn on or off the external field at a certain position (pixel). For instance when an electric field is applied and a dielectric alignment mechanism is operating $\epsilon\xi = \frac{\epsilon_0}{3}\Delta\alpha\mathbf{E}^2$. This is true in the case of nonpolar compunds where the dielectric constant

is essentially determined by a sum of the microscopic polarizability anisotropy $\Delta\alpha$ contributions.

The lattice is divided in regular arrays of sublattices where J has a chosen value making it is possible to control the effect of the field to produce the white/black patterns with a certain grey scale.

The updating of the lattice configurations is done according to a standard Metropolis Monte Carlo procedure [11], reorienting one spin at a time, so as to to ensure proper equilibration.

The display images can be obtained from the simulated lattice configurations by means of a standard matrix approach employed, for example, to simulate polarized optical textures both in Monte Carlo and continuum theory studies of polymer dispersed liquid crystals [8,12-15]. We describe each site in the display by a Müller matrix, so that the light beam travelling through a row of sites across the layers of the display 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 display 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.

SIMULATIONS AND RESULTS

In the twisted nematic display the aligned surfaces of the cell are orthogonally oriented (x and y directions) and the applied field **E** is directed along the z-axis. We assume $\xi > 0$, corresponding to a material with positive dielectric anisotropy. In the regions where the field is absent the effect of the boundary conditions tends to propagate inside the system producing a twisted nematic configuration. The application of a sufficiently strong field induces a change in the average orientation of the molecules on which it acts and produces an alignment along the field direction. An example of a display image as obtained from Monte Carlo simulations on a $50 \times 30 \times 10$ lattice at a reduced temperature $T^* = kT/\epsilon = 1.0$ is reported in Fig. 1 (left side).

With the MC technique it is also possible to investigate the molecular organisation and the ordering throughout the lattice, in particular on the different layers and in the two regions with ex-

ternal field *off* or *on*. The nematic ordering can be quantified by looking at the standard order parameter $\langle P_2 \rangle_\lambda$, obtained from the largest eigenvalue of the ordering matrix [7]. This quantity can also be calculated across the sample to investigate how the boundary layers, mimicking the effect of the aligning cell surfaces, influence the liquid crystal inside the lattice in the regions where the field is active or not [4].

It is convenient, however, to define and calculate in addition a specific microscopic quantity which expresses disordering from the ideal organisation inside the simulation cell. For the TN display we have found useful to calculate at each layer of the sample an *helical order parameter*, $< P_2 >_H$ defined as [4]:

$$< P_2 >_H = \frac{1}{N_L} \sum_{i=1}^{N_L} P_2(\mathbf{u}_i \cdot \mathbf{t}_i), \tag{3}$$

where N_L is the number of particles contained in the L-th plane, $\mathbf{u}_i$ is the orientation vector for the i-th spin and $\mathbf{t}_i$ is the ideal twist direction at the point i . This expresses disordering from a perfect twisted organization and is a maximum when all the particles lie parallel to the direction defined by the discretized helix between the bottom and top surfaces.

FIGURE 1 Optical images obtained by Monte Carlo simulations on $50 \times 30 \times 10$ lattice. (*Left*): Twisted nematic display, (*Right*): In-Plane Switching display. The applied field strengths are $\xi = 1$ and $\xi = -9$ respectively.

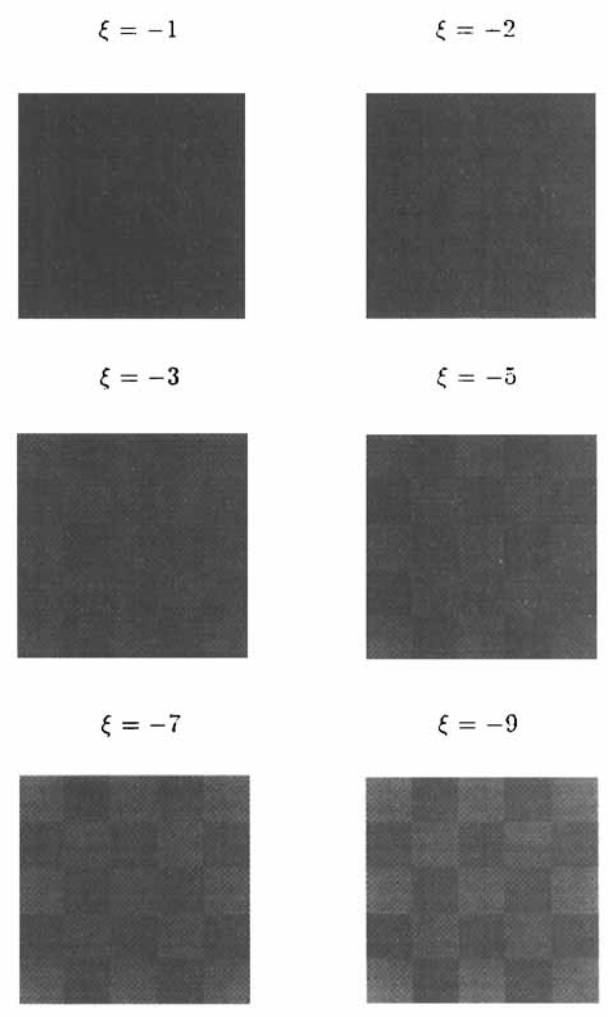

FIGURE 2 Effect of the increasing in the field strength on the simulated display images. These results were obtained by Monte Carlo simulations on a $10 \times 10 \times 10$ lattice for the In-Plane Switching case.

As a second example we consider a type of display recently proposed and based on the so called In-Plane Switching effect. In this device the cell surfaces are treated to induce a parallel alignment (x-direction) and the field acts only to the molecules belonging to an intermediate layer of the liquid crystalline material, which is in this case chosen to have a negative dielectric anisotropy.

The direction of the applied field is therefore parallel to the aligned surfaces but, due to the negative dielectric anisotropy now assumed, i.e $\xi < 0$, the molecules under the effect of the field tend to rotate by 90 degrees. Consequentely a twisted alignment is induced between this intermediate layer and the two aligned surfaces. Contrary to the previous case the light is trasmitted only where the effect of the field is non negligible. The background of the image is then black, see Fig.1 (right side). Since the electric field is applied only to one layer it is quite obvious that the strength of this external coupling has to be stronger, in comparison with the twisted nematic case, to overcome the effect of the anisotropic intermolecular potentials which tends to align the molecules one parallel to each other. The influence of the external coupling, through the parameter ξ in our model (eq. 2), on the simulated optical textures is shown in Fig. 2.

Also for this case it is possible to investigate the ordering inside the cell by calculating suitable order parameters. A particularly interesting one is the *field order parameter*, $\langle P_2 \rangle_E$, which quantifies the order of the system with respect to the field direction:

$$\langle P_2 \rangle_E = \frac{1}{N_c} \sum_{i=1}^{N_c} P_2(\mathbf{s}_i \cdot \mathbf{E}), \tag{4}$$

where N_c is the number of spins taken into account. Of course $\langle P_2 \rangle_E$ is maximum when all the molecules are directed along the field direction. This field order parameter can be calculated at the intermediate layer, containing the electrodes, and in well defined zones, determining for example $\langle P_2 \rangle_E^{ON}$ and $\langle P_2 \rangle_E^{OFF}$ to study regions where the field is active or not. The same type of calculations can be performed also for the other layers where the field is not directly applied, to investigate how the effect of the field propagates

across the simulated cell. In Fig. 3 we report these field order parameters calculated over the whole system. The results for the field order parameters $\langle P_2 \rangle_E^{OFF}$ and $\langle P_2 \rangle_E^{ON}$ as a function of field strength and position along the z axis are reported in Figs. 4 and 5. It is interesting to notice that the contrast between the black and white textures in the simulated optical images increases as the difference between $\langle P_2 \rangle_E^{OFF}$ and $\langle P_2 \rangle_E^{ON}$ increases.

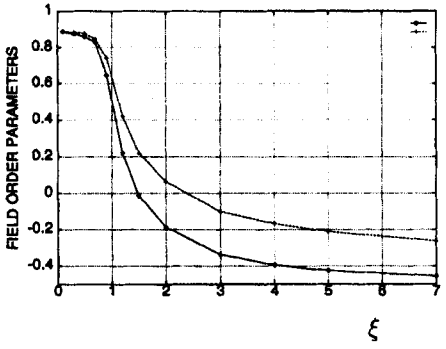

FIGURE 3 The order with respect to the field direction in the In-Plane Switching case for various field intensities obtained from MC simulations on a $10 \times 10 \times 10$ lattice at a reduced temperature $T^* = kT\epsilon = 1$. The order parameter $\langle P_2 \rangle_E^{ON}$ (*lower curve*) is calculated on all the molecules on which the field is applied while $\langle P_2 \rangle_E^{OFF}$ (*upper curve*) is for the molecules not directly addressed by the electric coupling.

As mentioned before the In-Plane Switching display requires a stronger field to obtain a sufficiently clear optical image. However, to force the formation of the twisted structure it is possible to act also on the anchoring at the aligned surfaces. In our model this can be easily realized modifying the hamiltionian by adding the following term which keeps into account the coupling with the

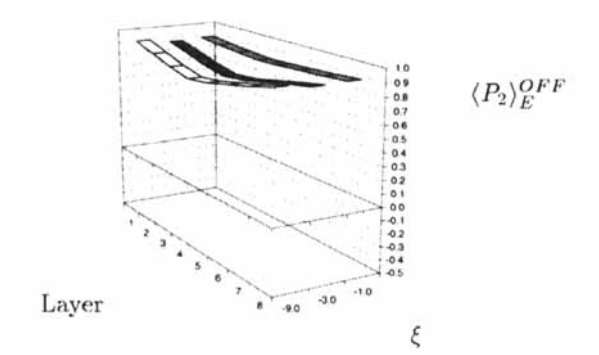

FIGURE 4 The field order parameter calculated for each layer in the regions where the field is **not** active as a function of field strength.

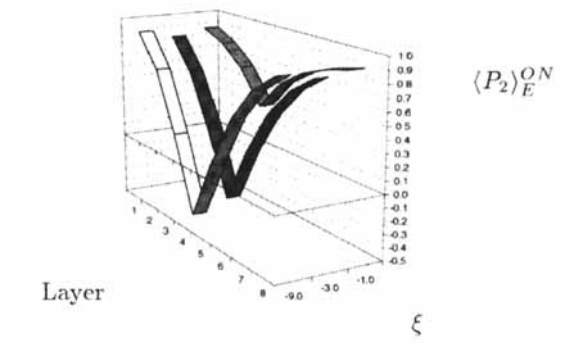

FIGURE 5 The field order parameter calculated for each layer in the regions where the field is active as a function of field strength.

particles placed at the fixed bottom and top surfaces:

$$U_s = -A_b \sum_i^{N_{bs}} \epsilon P_2(\cos\beta_{i,bs}) - A_t \sum_i^{N_{ts}} \epsilon P_2(\cos\beta_{i,ts}) \qquad (5)$$

FIGURE 6 The influence of the anchoring strength on the optical images. The textures have been obtained for a field strength of value $\xi = -5$ (see text) for different coupling with the aligned surfaces, i.e $A_b = A_t = 1$ (left), $A_b = 2, A_t = 1$(middle), $A_b = A_t = 2$ (right)

where N_{bs} and N_{ts} are the number of spins belonging to the bottom and top fixed oriented layers respectively. The strength of coupling with the surfaces is modulated by the parameters A_b and A_t.

In all the calculations presented above we have considered $A_b = A_t = 1$, i.e. the interactions with the surfaces were taken to be of the same strength of the interactions between the nematic molecules inside the sample. The influence of the anchoring on the performance of the display is shown in Fig. 6. It can be noticed that increasing the anchoring at the surface a lower field is required to obtain sufficiently defined images.

CONCLUSIONS

We have shown that Monte Carlo simulations could be a useful tool to investigate liquid crystal displays starting from simple intermolecular interactions. Our simulations are based on the simplest lattice potential proposed to describe nematic liquid crystals, i.e. the Lebwohl-Lasher one. In this model the molecules are considered to have uniaxial symmetry, and moreover the model generates equal elastic constants. A natural extension towards closer contact with reality could be to use a biaxial potential on a lattice [16] to keep into account the molecular biaxiality with the attendant expected difference in the elastic constants. The increase in computer power now makes it feasible also to use more realistic hamiltonians such as the Gay-Berne one [17]. However, this would imply much smaller samples than the ones that can be employed with lattices

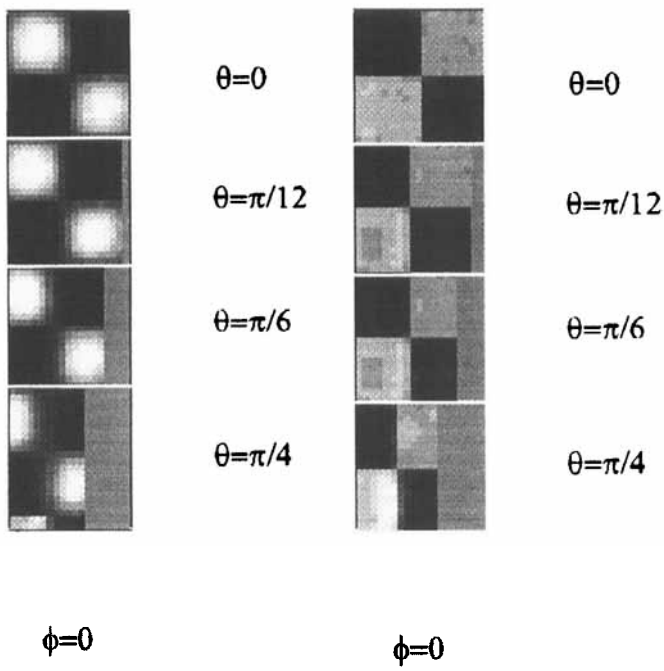

FIGURE 7 Simulated optical images obtained for different viewing angles. The angle Θ denotes the angle between the direction of the incoming light and the normal to the display surface. The results are for a Twisted Nematic Display (*left*) and an In-Plane Switching one (*right*).

and, as the functioning of displays relies essentially on purely orientational properties, it is probably still preferable to use lattices of very large sizes possibly including more details of technological interest like impurities in the nematic, defects at the surfaces and so on. In fact, as we have shown here, simple lattice spin models are sufficient to reproduce the basic features of the optics of different display types. Moreover a number of different conditions such as for example surface anchoring or viewing angle (*cf. Fig. 7*) can be investigated both qualitatively by looking at the optical textures

and quantitatively by defining contrasting ratios and suitable order parameters.

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