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# SIMULATIONS OF TOPOLOGICAL DEFECTS IN NEMATIC LIQUID CRYSTAL FILMS

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*We present a detailed computer simulation study of the formation and evolution of topological defects in thin 3D nematic films with schlieren geometry. The differences between the uniaxial and the biaxial case and the influence of the strength of anchoring to the surfaces are analyzed.*

*Keywords*: computer simulation; Monte Carlo; biaxial nematics; topological defects

## INTRODUCTION

Topological defects which appear in nematics confined between aligning surfaces and that are related, in particular, to the elastic properties of liquid crystals, have attracted a lot of interest from the scientific and technological points of view [1–3]. From the technological side the importance is mainly related to the application of liquid crystals to the development of displays and electro-optical devices [2]. From the basic research side the main interest is connected to the formation of various types of defects and to how these defects are related to the elastic and ultimately to the molecular properties of the material. Experimentally a great amount of work has been performed by various groups [4,5]. Theoretically the approach has normally been based on continuum elastic theories [2,3], although recently computer simulations have also been applied to study the involved phenomena [6–9].

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Here we aim to present a detailed simulation study of the Schlieren textures in a nematic film, textures which occur when at the top and bottom surfaces the local director orientation is isotropically distributed on the plane. The effect of the thickness of the film and of coupling strength with the aligning surfaces together with the differences between the uniaxial and biaxial cases are investigated.

## THE SIMULATION MODEL



The simulation model adopted here is a generalization to biaxial molecules [10] of the Lebwohl-Lasher (LL) lattice one [11] for nematics. The model is clearly limited to the treatment of properties related to orientational, as opposed to positional, order, but otherwise the restriction of having the $N$ molecules fixed at the sites of a cubic lattice does not affect the orientational and phase transition behaviour of the liquid crystal [10]. The rich phase diagram of a biaxial nematic system with isotropic, uniaxial and biaxial phases can be derived by the hamiltonian [10]:

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

where $\mathcal{F}, \mathcal{S}$ 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. A bulk sample [10] is modelled letting $J=0$ and imposing periodic boundary conditions. The interaction between the particles is through the second rank attractive pair potential:

$$\begin{aligned}\Phi_{ij} = -\varepsilon_{ij}\{&P_2(\cos\beta_{ij}) + 2\lambda[R^2_{02}(\omega_{ij}) + R^2_{20}(\omega_{ij})]\\ &+ 4\lambda^2 R^2_{22}(\omega_{ij})\}\end{aligned} \tag{2}$$

where $\varepsilon_{ij}$ is a positive constant, $\varepsilon$, for nearest neighbour molecules $i$ and $j$ and zero otherwise, $\omega \equiv (\alpha, \beta, \gamma)$ is the set of Euler angles specifying molecular orientations and $R^L_{mn}$ are symmetrized combinations of Wigner functions [12]. The biaxiality parameter $\lambda$ takes into account the deviation from cylindrical molecular symmetry: when $\lambda$ is zero, the biaxial potential reduces to the LL one, while for $\lambda$ different from zero the particles tend to align not only their major axis, but also their short one.

We have studied systems of size $N = L \times L \times (d+2)$, where $d \ll L$ is the thickness of the nematic film, at temperatures deep in the nematic phase, $T^* \equiv k_B T/\varepsilon = 0.1$ and $T^* = 0.4$. The tangential boundary conditions at the two horizontal surfaces were implemented by fixing random$(x, y)$ in-plane orientations of the longest molecular axes (director $\mathbf{n}$) and a random alignment of the orthogonal directors $l$ and $m$. At the

other four lateral faces of the system we leaved free boundaries, i.e. empty space. 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 [13]. Polarizing microscope textures were simulated assuming the spins to act as retarders on the light propagating through the film by means of a Müller matrix approach described elsewhere [7].

## SIMULATION RESULTS

As mentioned before we have investigated uniaxial and biaxial systems with different thickness and coupling strength at the surfaces and we report in the following the various cases studied.

### Uniaxial Nematic Films

The first case examined is a uniaxial nematic film of size $120 \times 120 \times (8+2)$ with an interaction at the orienting surfaces of the same strength as that inside the liquid crystal (i.e. $J = 1$).

The optical parameters employed were: film thickness $d = 5.3\,\mu m$, ordinary and extraordinary refractive indices $n_o = 1.5$ and $n_e = 1.66$, and light wavelength $\lambda_o = 545\,\text{nm}$. The resulting simulated Schlieren textures as observed between crossed polarizers after an increasing number of evolution cycles are presented in Figure 1 and show the formation and coarsening of the defects. It is clear from the images that a network of defects with four brushes (strength $k = |1|$) and two brushes (strength $k = |1/2|$) is formed just after a few thousands of MC lattice updates (cycles).

The four brushes defect show the ring characteristic of an escaping director configuration [14] with the black circular area corresponding to the angle where in, the continuous change from planar orientation at the surface to homeotropic inside the film, the retardation is compensated out (see Fig. 4 later). This type of defects should be particularly evident observing the film between circular polarizes of opposite handedness and in Fig. 2 we present these textures. The $k = |1|$ disclinations are less stable than the $k = |1/2|$ ones and disappear as it is clearly evident from Figure 2 where we see the annealing out of the $k = |1|$ defects. e.g. by combination of opposite sign disclinations shown in Figure 3. The use of circular polarizers seemingly not often used in this context appears particularly suitable to detect the four brushes defects which have circular symmetry.

Since real uniaxial nematic films present in the Schlieren geometry mainly defects of strength $k = |1|$ we have examined if the disappearing of

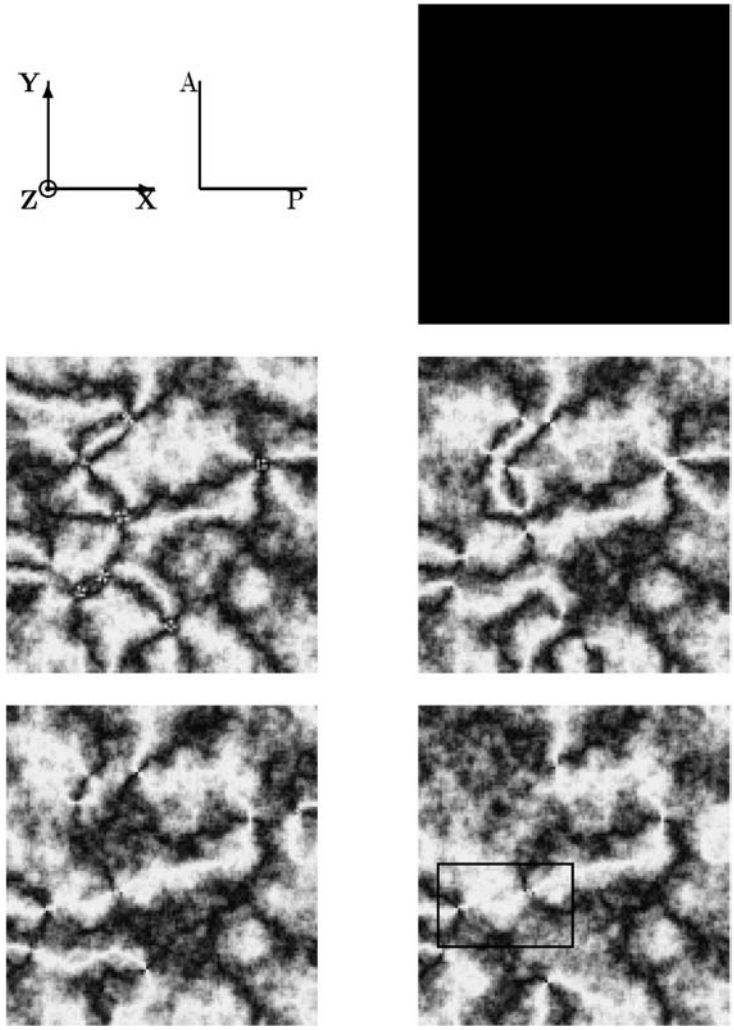


**FIGURE 1** Schlieren textures of a uniaxial nematic film at the reduced temperature $T^* = 0.1$. The first frame indicates the observer point of view of the $120 \times 120 \times 10$ system and the orientation of the crossed polarizers (P,A) while the others (from top right to bottom right) show the optical images taken after 0, 5000, 10000, 20000, and 60000 MC cycles.

two brushes defects is due to the fact of having particularly thin films. We have thus doubled the thickness (to $d = 16$) of the simulation sample maintaining all the other parameters to the same values of the previous

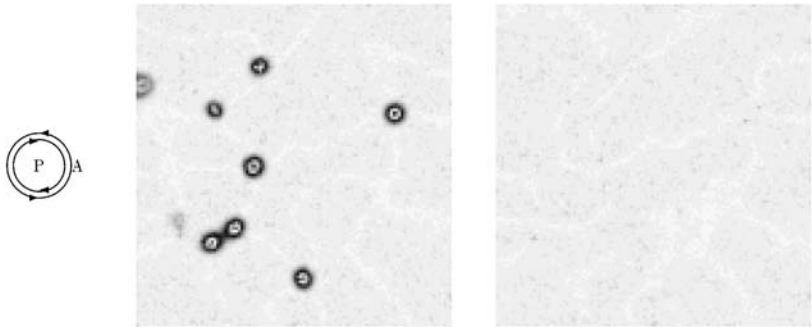


**FIGURE 2** Optical textures of the same system of in Figure 1 as observed between circular polarizers (P,A) after 5000 and 10000 MC cycles.

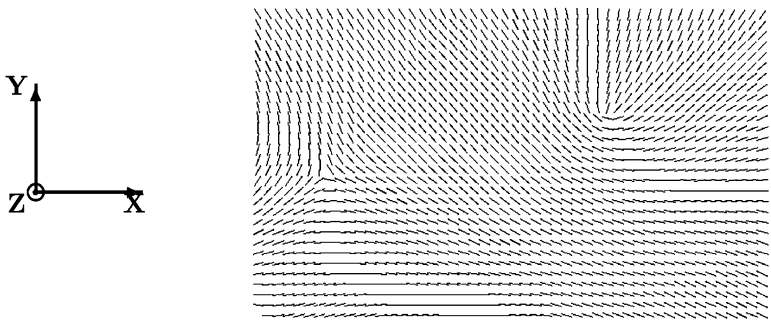


**FIGURE 3** Snapshot of a horizontal section (middle layer) of the portion of the system evidenced in Figure 1 (last frame) where it is possible to see the two disclinations of strength $k = \pm 1/2$.

case (i.e. $J = 1$ and $T^* = 0.1$). In Figure 4 we present the results for this "thick" $120 \times 120 \times (16 + 2)$ system and we can observe that only $k = |1|$ type disclinations are present in this case. At the centre of these defects we have the escape in the third dimension as can be seen from the snapshots shown in Figure 4.

One of the main effects of increasing sample thickness is that of reducing the importance of the anchoring boundaries. We have thus also analyzed the influence of the strength of coupling to the surfaces by reducing the value of the anchoring parameter $J$, to $J = 1/2$. Simulating in this case again a thin $120 \times 120 \times (8 + 2)$ film we obtain results similar to those just shown for the system two times thicker and with $J = 1$ (see Fig. 5). Increasing the temperature to $T^* = 0.4$ we obtain, probably due to the fact that the molecules are now more disordered, interesting patterns where it

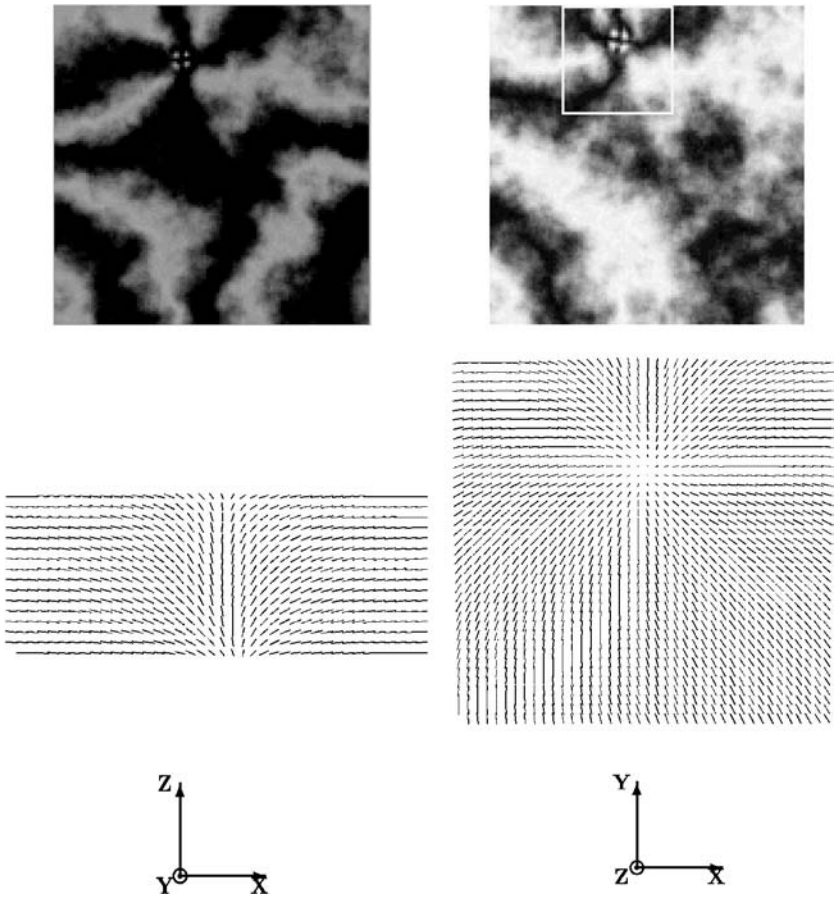


**FIGURE 4** Optical textures of a thicker ($120 \times 120 \times 18$) uniaxial nematic system at $T^* = 0.1$ and $J = 1$ after 20000 and 60000 MC cycles (*Top*). Snapshots of a vertical section and of the horizontal middle layer of the region indicated above containing a $k = |1|$ type stable disclination.

is possible to observe the annihilation of two defects of different sign (see Figs. 6 and 7).

## Biaxial Nematic Films

A particularly interesting case is the films formed by biaxial liquid crystal molecules. Biaxial nematics, in fact, have been the subject of a wide number of investigations in the last few years [15]. Their existence have

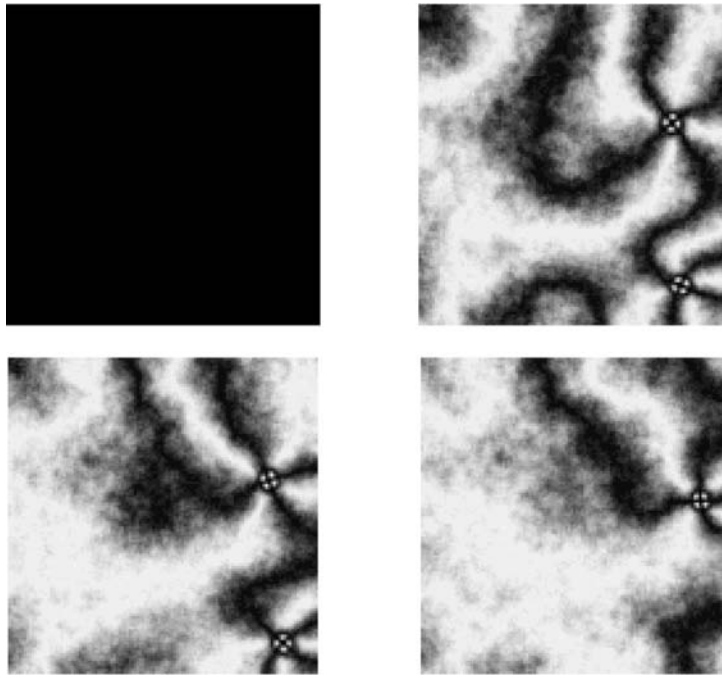

**FIGURE 5** Evolution of the optical textures for a $120 \times 120 \times (8+2)$ system with a weak coupling with the surfaces ($J = 1/2$) at 0, 10000, 20000 and 60000 MC cycles (from top left to bottom right).

been predicted by theories [15] and computer simulations [10] while no complete experimental evidence is found yet. In particular NMR investigations of suitably deuterated mesogens proposed as candidates to generate biaxial nematics have not shown the expected phase biaxiality [16]. This negative results may well be due to the fact that the nematics had been incorrectly assigned in the first place but could also, conceivably, be due to the not very high sensitivity of what is otherwise a very reliable technique. There has therefore been much interest in developing some other highly sensitive diagnostic techniques, in order to cross check the phase biaxiality. Recently Chandrasekhar et al. [17], following an idea put forward by de Gennes [18], have tried to identify their biaxial nematics looking at the topological defects which are formed in the Schlieren geometry. Their hypothesis is that biaxial nematics would present only stable defects with two brushes, i.e. $k = |1/2|$.

In a separate study [8] we have examined the problem by a combination of MC simulations and continuum theory. Here we report further simulation studies. We have then tried to verify the de Gennes' conjecture by simulating

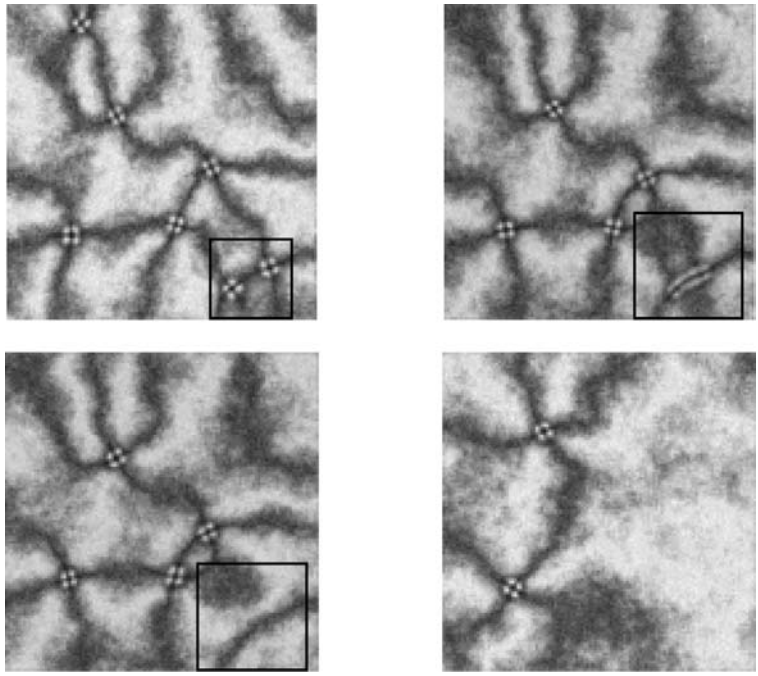

**FIGURE 6** Evolution of the optical textures for a $120 \times 120 \times (8+2)$ film with a weak anchoring to the surfaces ($J = 1/2$) at $T^* = 0.4$. The images are taken after 5000, 8000, 9000 and 60000 MC cycles (from top left to bottom right). The square indicates the annihilation of two disclinations with opposite sign.

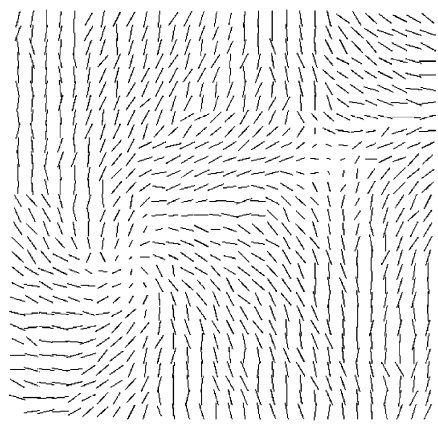

**FIGURE 7** Snapshots of the middle layer of the system portion shown in Figure 6 (first frame) with the annihilation of the two defects.

a biaxial model with molecular biaxiality $\lambda = 0.2$ and $\lambda = 0.25$ at a reduced temperature $T^* = 0.1$. We have first checked that our material is in a biaxial phase by monitoring the biaxial order parameters [10] which are non zero only in that case. In the biaxial case we have three refractive indices which have to be parameterized with the molecular biaxiality $\lambda$. For the two values of biaxiality we have chosen the following values: $\lambda = 0.2$, $n_x = 1.54$, $n_y = 1.51$, $n_z = 1.61$; $\lambda = 0.25$, $n_x = 1.55$, $n_y = 1.52$, $n_z = 1.59$. From the results for a $120 \times 120 \times (8 + 2)$ film shown in Figure 8 we can notice that the Schlieren textures are similar to those experimentally observed by Chandrasekhar [17] and other researchers [19]. The four brushes defects are less frequent than the $k = |1/2|$ disclinations. After some thousands of MC cycles the $k = |1|$ defects disappear by splitting in pairs of $k = \pm 1/2$ lines (see Fig. 9). A continuum theory treatment discussing the limits of stability



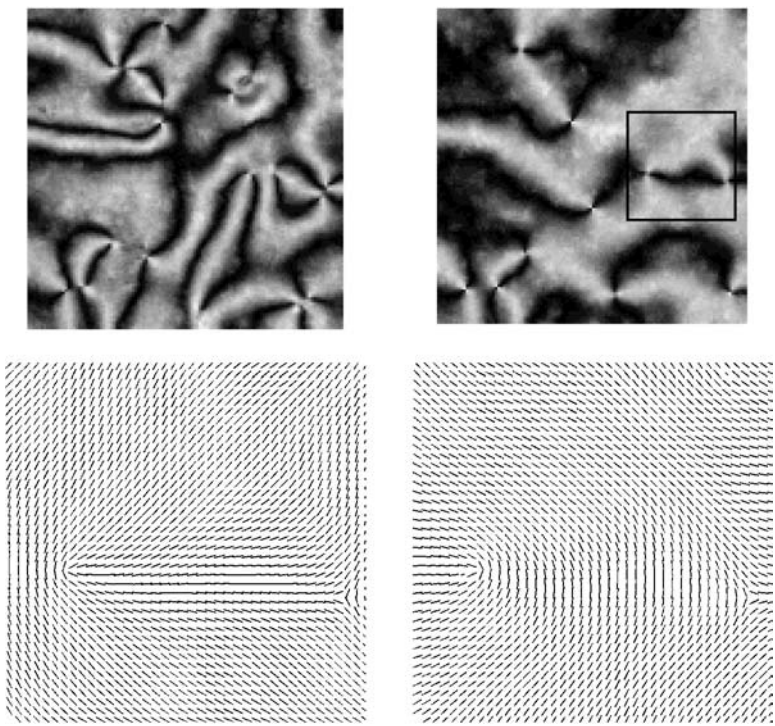

**FIGURE 8** Results for a $120 \times 120 \times (8 + 2)$ biaxial film. The molecular biaxiality is $\lambda = 0.2$, the coupling with the surfaces $J = 1$ and $T^* = 0.1$ (*Top*). The images are taken after 5000 (*left*) and 60000 (*right*) MC cycles. (*Bottom*) Snapshots of the middle layer of the enhanced portion of the lattice with tow $k = |1/2|$ disclinations: long (left) and short (right) molecular axes.

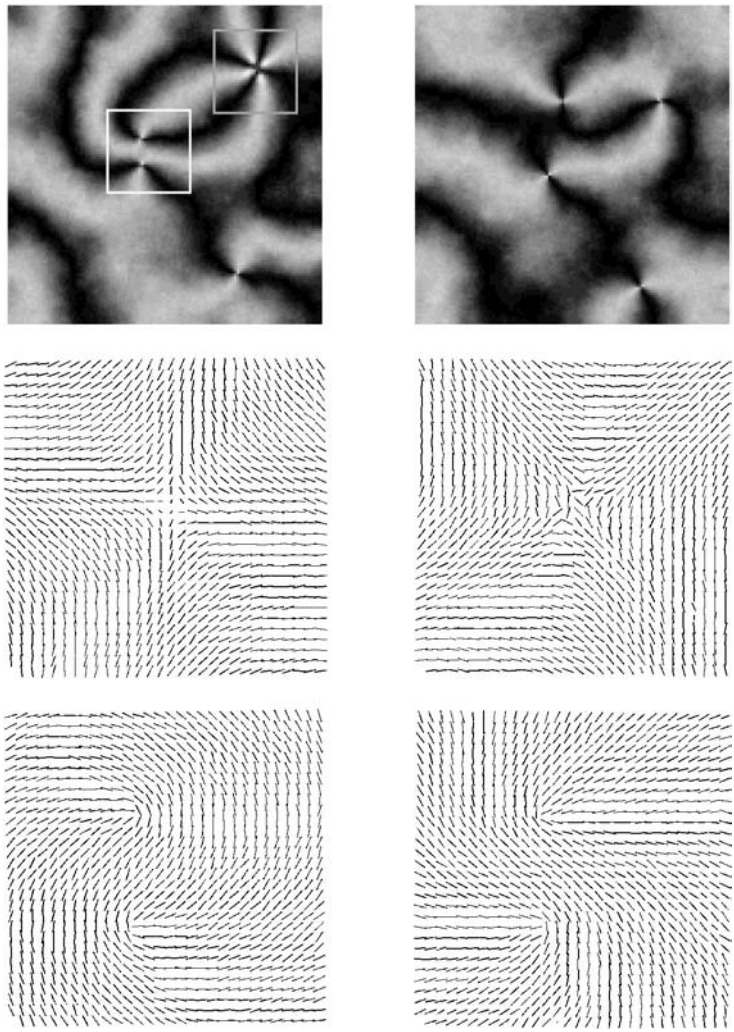

**FIGURE 9** Results for a $120 \times 120 \times (8+2)$ biaxial film. The molecular biaxiality is $\lambda = 0.2$, the coupling with the surfaces $J = 1/2$ and $T^* = 0.1$. (*Top*) The images are taken after 13000 (*top left*) and 60000 (*top right*) MC cycles. The other frames show snapshots of the middle layer of the portions of the system evidenced with a grey and a white square in the top left frame. In these regions a $k = |1|$ (*center*) and a $k = |1/2|$ (*bottom*) defect are present. The long molecular axes are shown on the left and the short ones on the right.

of the different types of defects for uniaxial and biaxial nematics has been given elsewhere [8]. Also in the biaxial case we have varied the thickness of the film and the strength of the coupling with the surfaces. All the simulation results confirm that, at least for our parameterization, the only stable disclinations for the biaxial case are those of strength $k = |1/2|$.

## CONCLUSIONS

We have presented a detailed simulation study of thin 3D films of uniaxial and biaxial nematics with tangential boundary conditions to contribute to the current debate on the existence of biaxial nematic phases and the possible differences in the Schlieren textures of uniaxial and biaxial nematics. The simulations in fact show for our case distinct differences in structure and evolution of topological defects. In the uniaxial films, defects of strength $k = |1|$ are point defects that bear no bulk singularity and disappear by annihilation with each other. In the biaxial films, $k = |1|$ defects are true singular bulk disclinations that split into pairs of $k = \pm 1$ lines.



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