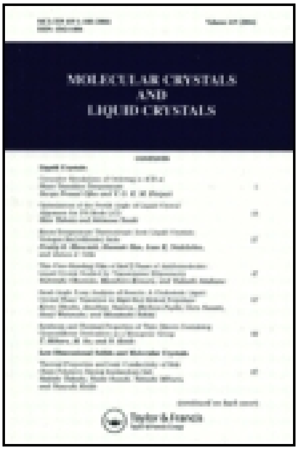


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# Numerical Simulations of Three Dimensional Liquid Crystal Cells

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# Numerical Simulations of Three Dimensional Liquid Crystal Cells

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Director fields and electrostatic potential functions for three dimensional liquid crystal cells have been calculated numerically by solving the discretized Frank-Oseen equations for a nematic liquid crystal with a fast nonlinear multigrid algorithm on an adaptive grid. All elastic constants, including the $k_{24}$ term and an anchoring coefficient at the surfaces, were taken into account. Two configurations with different boundary conditions were investigated: multidomain cells and hybrid aligned films

*Keywords:* topological defects

## INTRODUCTION

Three dimensional director fields attract considerable interest now, because display technology has become more and more complex and, therefore, the features of liquid crystal (LC) cells cannot be modeled any more by one or two dimensional geometries. This is also due to the fact that the director field in a nematic LC display can exhibit topological defect structures. For such reasons we performed 3D calculations for static director fields corresponding to two particular situations.

One problem of liquid crystal displays, which cannot be solved without applying complex techniques (e.g. thinfilm transistor techniques) is the dependence of the contrast on the viewing angle. Multidomain cells reduce this dependence in a straightforward way. The geometry is similar to twisted nematic cells[8], but left- and right-handed helices alternate as in a checkerbord pattern. This may be achieved by a striped anchoring scheme of the director (other realisations are also possible, however): the pretilt is constant on both cover glasses, whereas the pretwist alternates from one stripe to the next between opposite directions parallel to the stripes. The stripes of the cover glasses are orientated perpendicular to each other[1], resulting in four pretwist combinations between top and bottom. A certain handedness of the helix is preferred for each of the four combinations, due to a lower splay energy density. The arrangement of the four combinations results in the checkerboard pattern of the helices. Between the domains line defects should appear, as helices of different handedness do not match.

Our second example is not yet realized in displays. Hybrid aligned nematic films (HAN) possess hybrid boundary conditions. The liquid crystal is situated on an isotropic fluid, where the director may only rotate within the surface (planar anchoring). The upper boundary is left free, thereby achieving a homeotropic anchoring for certain types of molecules. These cells show many different and complex defect structures[3,4,5].

## THEORETICAL AND NUMERICAL ASPECTS

To calculate static configurations of director fields we search for minima of the nematic elastic and electric energy whose density reads

$$\begin{aligned} f^{\mathrm{vol}}_{\mathrm{elast}} = & \frac{1}{12}(3k_{22} - k_{11} + k_{33} - 6k_{24})Q_{ij,k}Q_{ij,k} + \frac{1}{2}(k_{11} - 2k_{24})Q_{jk,k}Q_{jl,l} \\ & + \frac{1}{2}(2k_{24} - k_{22})Q_{jk,l}Q_{jl,k} - \frac{2\pi}{p}k_{22}\epsilon_{jkl}Q_{jm}Q_{km,l} \\ & + \frac{1}{4}(k_{33} - k_{11})Q_{jk}Q_{lm,j}Q_{lm,k} \\ & - \frac{1}{2}\epsilon_0(\epsilon_{\parallel} - \epsilon_{\perp})\left(\frac{\epsilon_{\parallel} + 2\epsilon_{\perp}}{3(\epsilon_{\parallel} - \epsilon_{\perp})}\delta_{ij} + Q_{ij}\right)U_{,i}U_{,j}. \end{aligned} \tag{1}$$

Here

$$Q_{ij} = n_i n_j - \frac{1}{3}\delta_{ij}$$

is the uniaxial alignment tensor. $k_{11}$, $k_{22}$, and $k_{33}$ are the elastic constants of splay, twist and bend deformations. $k_{24}$ describes the saddle splay elastic surface term. $p \neq 0$ is the intrinsic cholesteric pitch, in our calculations we set $\frac{2\pi}{p} = 0$ (nematic).

To investigate the elastic deformations due to a voltage $U$, we need the dielectic constant parallel ($\epsilon_{\parallel}$) and perpendicular ($\epsilon_{\perp}$) to the director. $\epsilon_0$ is the dielectric constant of the vacuum.

As stated above, topological defects usually occur in the nematic phase. However, we neglect the energy content of their cores, assuming that the finest grid employed is coarse compared to the dimension of the defect cores. Thus, in our considerations only distortions of the director field contribute to the elastic energy. This causes some peculiarities in the case of the hybrid aligned film, as we shall see below.

The surface anchoring of the director in case of the multidomain cell is modeled by the potential

$$f_{\text{surf}} = -\frac{1}{2}c\,(\mathbf{n}\cdot\mathbf{n}_{\text{pre}})^2\,.$$

For the HAN cells we use an extended Rapini-Papoular[7] potential ($c_\phi = 0$ on the lower boundary):

$$f_{\text{surf}} = \frac{1}{2}\sin^2(\theta-\theta_{\text{pre}})\left[c_\theta + c_\phi \sin^2(\phi-\phi_{\text{pre}})\right],$$

where $c$, $c_\phi$, $c_\theta$ are the anchoring constants. $\theta$ and $\phi$ are the spherical coordinates of the director.

The minimum of this energy density is found by solving the discretised corresponding Euler-Lagrange equations for the director tilt and twist angles $\theta$ and $\phi$ and for the electrostatic potential $U$ with an adaptive multigrid method[6].

Finally we calculate the intensity of the light transmission for the case of perpendicular incident with a $2 \times 2$ Jones matrix method[9].

## MULTIDOMAIN CELL WITH TWO DISCLINATIONS

Here we present our numerical investigations of a multidomain structure consisting of two right- and two left-handed helices as described above. The material parameters were taken from [1], assuming strong surface anchoring. The light transmission (Fig. 1a) shows two dark lines representing two disclinations. If the voltage is decreased, the line defects disappear and the transmission is almost homogeneous (Fig. 1b).

A quantitative analysis is shown in Fig. 1. Obviously there are two different configurations, depending on the voltage and the pretilt at the surface. This fact can be explained when considering the director field of the homogeneous structure. Two of the domains should have changed their helix to the unfavoured handedness, increasing the splay energy. This is indeed the case, as shown in Fig. 3a where two of the four domains reveal a higher splay energy. If the voltage is high enough, the multidomain configuration is achieved, and the splay energy is the same for helices of right and left handedness (Fig. 3b). The specific feature of the configuration phase diagram depends on the elastic constants and the anchoring strength. It may also vary, if the core energy is not neglected any more.

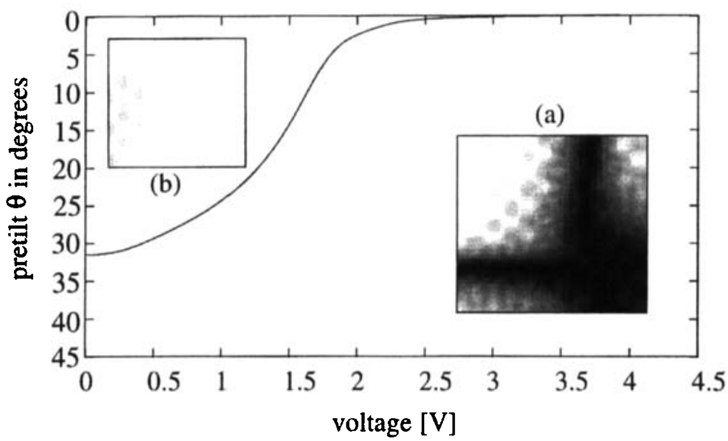



FIGURE 1 Configuration phase diagram of the multidomain cell. For low voltages and low pretilts (parallel orientation for $\theta = 0$) the disclinations disappear. (a) Transmission of a multidomain cell with disclinations at 2 V and with $\theta = 10°$. The cell contains two orthogonal line disclinations. (b) The transmission at 1 V and with $\theta = 4°$ is homogenous, although the boundary conditions are not changed.

## HYBRID ALIGNED FILM WITH SURFACE POINT DEFECT

The simplest defect of a hybrid aligned film is a surface defect of strength $S = +1$. This defect is located on the lower surface of the liquid crystal, where the isotropic fluid is situated. The results of the simulation are shown in Fig. 4. The anchoring on the lower surface was hard in $\theta$, free in $\phi$. The other surface was anchored hard and homeotropic. The film is $6\mu$m high, the lateral dimensions were varied from $6\mu$m to $600\mu$m without any change in the director field configuration. Two gaussian curvatures are possible (Fig. 4a and 4b), the transmission is almost the same in both cases (Fig. 2), as the strength of the defect is the same.

If the absolute values of the splay energy are taken into account, the two configurations with different curvature are equivalent. Only the maximum value of the energy near the core of the defect is different.

When all directors may rotate freely in the surface (anchoring hard in $c_\theta$), we observed a splitting of the defect into two defects of strength $S = \frac{1}{2}$, a fact that is not observed in the experiment. Obviously the defect does not move on an intermediate lattice point by itself during the numerical relaxation. After tilting the director in the middle normal to the surface of the cell, the defect of strenght $S = 1$ remained stable, but onother director of the surface was also tilted out of the plane. Obviously the defect is located very near to this middle director, so that the limit of the continuum mechanical description is reached.

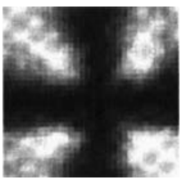
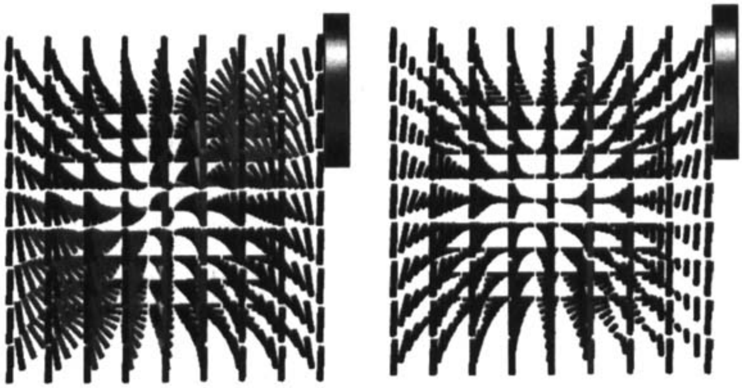


FIGURE 2 The light transmission of the director field (a) and (b) is almost the same. The four brushes show the existence of a point defect of strength $S = 1$.

Summing up, we presented threedimensional directorfields of to different boundary conditions. Multidomain cells are used to decrease the dependence of the contrast on the viewing angle. As shown in the konfiguration phase diagram a mimimum pretilt is needed therefor. For the hybrid aligned films we showed two equivalent gaussian curvatures of a surface defect of strength $S = 1$.



(a) (b)

FIGURE 3 (a) Director field of the multidomain cell without disclinations ($6\mu m \times 6\mu m \times 6\mu m$). The director is shown as a cylinder. The colors encode the splay energy. Light blue areas are of higher splay energy than violet areas. Here the two anchored layers of directors are the top and bottom layer. ($U = 1V$, $\theta = 4°$). The legend is linear, a temperature-like coloring is used (in units of $J/\mu m^3$): 0 (dark blue), 0.031 (red). (b) Director field of the multidomain cell with disclinations ($U = 2V$, $\theta = 4°$). Legend: 0.00 (dark blue), 3.60 (red).

(See Color Plate XXI at the back of this issue)

(a) (b)

FIGURE 4 Director configurations of a hybrid aligned film: positive (a) and negative (b) Gaussian curvature is possible. The colors encode the splay energy. Legend (in units of $J/\mu m^3$): (a) 0.00 (dark blue), 3318 (red) and (b) 0.00 (dark blue), 2682 (red).

(See Color Plate XXII at the back of this issue)

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