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Computer Simulations of the π-Cell

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We present an algorithm for the numerical calculation of the static and dynamic behavior of nematic cells. Based on the tensorial description of the alignment, our algorithm preserves the nematic symmetry, i.e. the equivalence of **n** and **−n** which is essential not only for the occurrence of disclinations but also for the transition between topologically different aligned states. We specifically take the usual operating mode of electrooptical devices—a prescribed voltage rather than a prescribed field strength—into account.

Here, the π-cell is examined by computer simulation. The results, compared to experimental data, indicate reliability with respect to the Frank elasticity. The relaxation times are in good agreement with the experiment as long as backflow is negligible.

In addition, we predict conditions for the two-frequency control of the π-cell, which has not yet been realized in experiments.

Keywords: theory, orientational dynamics, computer simulation

BASIC EQUATIONS

We assume uniaxial alignment, which is described by an alignment tensor $a_{\mu\nu} = S \cdot \overleftrightarrow{n_\mu n_\nu}$. The symbol $\leftrightarrow$ refers to the symmetric traceless part of a tensor, S is the Maier-Saupe order-parameter and **n** the director, with $n_\mu n_\mu = 1$. The elastic energy (Frank/Oseen) in terms of the alignment tensor is

$$f_d = \frac{A}{4}(\nabla_\lambda a_{\mu\nu})(\nabla_\lambda a_{\mu\nu}) + \frac{B}{2}(\nabla_\nu a_{\mu\nu})(\nabla_\lambda a_{\mu\lambda}) + \frac{C}{4} a_{\lambda\kappa}(\nabla_\lambda a_{\mu\nu})(\nabla_\kappa a_{\mu\nu}) \quad (1)$$

where

$$\begin{aligned} A &= K_2 + (K_3 - K_1)/3 \\ B &= K_1 - K_2 \\ C &= K_3 - K_1 \end{aligned} \quad (2)$$

In case of uniaxial alignment this energy coincides with the usual Frank free energy, see [4], p.93. The orientational dynamics[1] for a constant order parameter S is [1]

$$a_{\kappa\nu} \cdot \varepsilon_{\lambda\kappa\mu} \left(\gamma_1 \frac{\partial a_{\mu\nu}}{\partial t} - \nabla_\lambda \frac{\partial f_d}{\partial a_{\mu\nu,\lambda}} - F_{\mu\nu} \right) = 0. \tag{3}$$

Here, flow processes are neglected and $F_{\mu\nu} = \Delta\varepsilon E_\mu E_\nu$ for a prescribed electric field. For nematic cells, one-dimensional spatial dependence may be assumed; we choose x as the direction perpendicular to the nematic layer. This allows use of Deuling's solution for a prescribed voltage. In this case, $F_{\mu\nu}$ is replaced by $E_o^2 \left(\varepsilon_{\text{eff}} \cdot \overline{\varepsilon_{\text{eff}}^{-1}} \right)^{-2} \Delta\varepsilon\delta_{x\nu}\delta_{x\mu}$, where $\varepsilon_{\text{eff}} := \varepsilon_{\text{iso}} + \Delta\varepsilon a_{xx}$ is the effective dielectric permittivity, and E_o the vacuum field strength caused by the applied voltage U.

THE NUMERICAL ALGORITHM

To maintain the nematic symmetry, one has to proceed as follows:

1. Discretize the tensorial equation on a uniform mesh.
2. Project the tensorial equation onto the director, i.e. multiply by **n**.

This leads to a "tensorial" algorithm in terms of the director. Different versions are possible. Simple example: one-coefficient-approximation ($B = C = 0$), prescribed electric field.[2]

$$n_\mu^{\text{new}} = \lambda\{\overline{n_\mu n_\nu} + \beta\hat{E}_\mu\hat{E}_\nu\}n_\nu \tag{4}$$

where $\beta = \Delta\varepsilon \cdot (\pi\delta x/L\ E/E_{\text{fred}})^2$ and λ such that $n_\mu n_\mu = 1$. The bar denotes the average over the $2d$ nearest neighbors (d is the dimension of the problem), and L is the cell thickness. Note that the action of the nematic environment is of the same tensorial type as the action of the external field.

For the computer simulations of the π-cell, however, only x-dependence and $K_1 = K_3$ was assumed. This leads to the following algorithm which performs one time step of length δt on the NLC (the superscripts + and − denote the neighbors above and below):

$$\begin{pmatrix} n_x^{\text{new}} \\ n_y^{\text{new}} \\ n_z^{\text{new}} \end{pmatrix} = \lambda \left\{ \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} + \alpha \begin{pmatrix} n_x^+ s^+ + n_x^- s^- - 2n_x \\ K_{21}\,[n_y^+ s^+ + n_y^- s^- - 2n_y] \\ K_{21}\,[n_z^+ s^+ + n_z^- s^- - 2n_z] \end{pmatrix} + \alpha\beta \begin{pmatrix} n_x \\ 0 \\ 0 \end{pmatrix} \right\}. \tag{5}$$

Here, K_{21} is the ratio of the elastic coefficients K_2/K_1, and $s^\pm = n_\mu n_\mu^\pm$ is the inner

[1] Unlike the more general term "alignment dynamics," this refers to pure rotations of the alignment tensor. Mathematically, the orientational part is extracted by the "cross product."

[2] For details, see Reference 2.

product of the director and its appropriate neighbor. The factors s make the difference between the vectorial and the tensorial calculus. If one would perform the projection onto the director prior the discretization, the only difference would be that s would not appear. Just by these factors, antiparallel neighbors are treated like parallel ones. The scaling factor λ has to be determined at every grid point. The dimensionless coefficients α and β are

$$\alpha = \frac{K_1 \delta t}{\gamma_1 \delta x^2}; \qquad \alpha\beta = \frac{U^2 \Delta\varepsilon \delta t}{\gamma_1 L^2} \cdot \left(\varepsilon_{\text{eff}} \overline{\varepsilon_{\text{eff}}^{-1}}\right)^{-2} \tag{6}$$

By choosing the proper value for α, one can control the speed of the iteration, i.e. the time resolution.[3]

THE π-CELL

The π-cell is characterized by parallel but oppositely tilted boundary conditions. This geometry allows[4] two untwisted steady states which are topologically different. This fact may be useful for multiplexing. Figure 1 shows these states. The vectorial calculus yields either one of these configurations as the unique twist-free solution of the appropriate steady-state condition[5] depending on the choice of the polarity of the boundary vectors. Therefore, it is not possible to describe the switching process between these two states within the framework of the director calculus, except by a boundary reversal, which should not affect the physical state. In contrast, our tensorial algorithm allows both of the states (plus disclinations, if two and three-dimensional simulations are performed) and is independent of the polarity of any director; the final state depends only on the initial state.

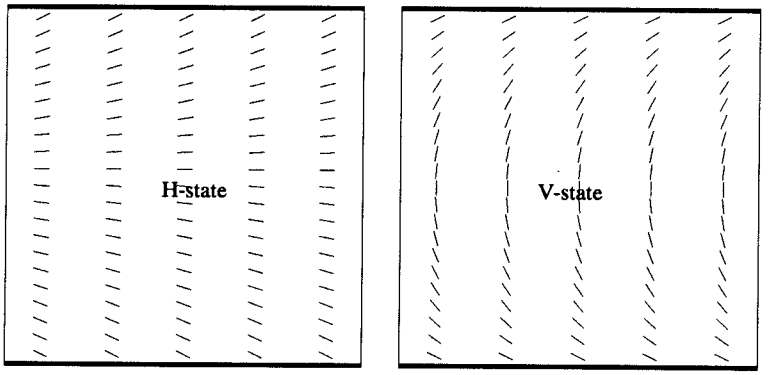

FIGURE 1 The equilibrium configurations of a π-cell. Here and in the Figures below, the results of the one-dimensional calculations are, for clarity, extended to two dimensions.

[3] A limit for the iteration speed is given by the condition that the components of the directors must not change their signs while performing one time step.

[4] Besides a theoretically infinite number of twist configurations.

[5] E.g. the Euler-Lagrange equation $\Delta\mathbf{n} = 0$, $\mathbf{n}^2 = 1$ for $K_1 = K_3$, see Equation [4].

Two-Frequency Control

Use a two-frequency-mixture to switch between the two states [3]. At the low frequency ($\Delta\varepsilon > 0$) the electric field causes the directors to align vertically. At the high frequency ($\Delta\varepsilon < 0$) the electric field should push the director field into the H-state. As the experimentalists reported, this did not work. Instead of the H-state, an unstable twist-state established, which decayed into the initial V-state when the voltage was turned off. Four stages of a computer simulation of the corresponding setup, performed as a quasi-equilibrium process, are shown in Figure 2. The simulation is in agreement with the experimental results. Encouraged by this coincidence, we performed a series of "computer-experiments" including different values of K_1/K_2 and found conditions which avoid the twist-state and favor the transition to the H-mode.

Results

First of all, the switching is a non-equilibrium process. We used triangle-shaped pulses. One series of simulations, which examine the influence of the slope of the

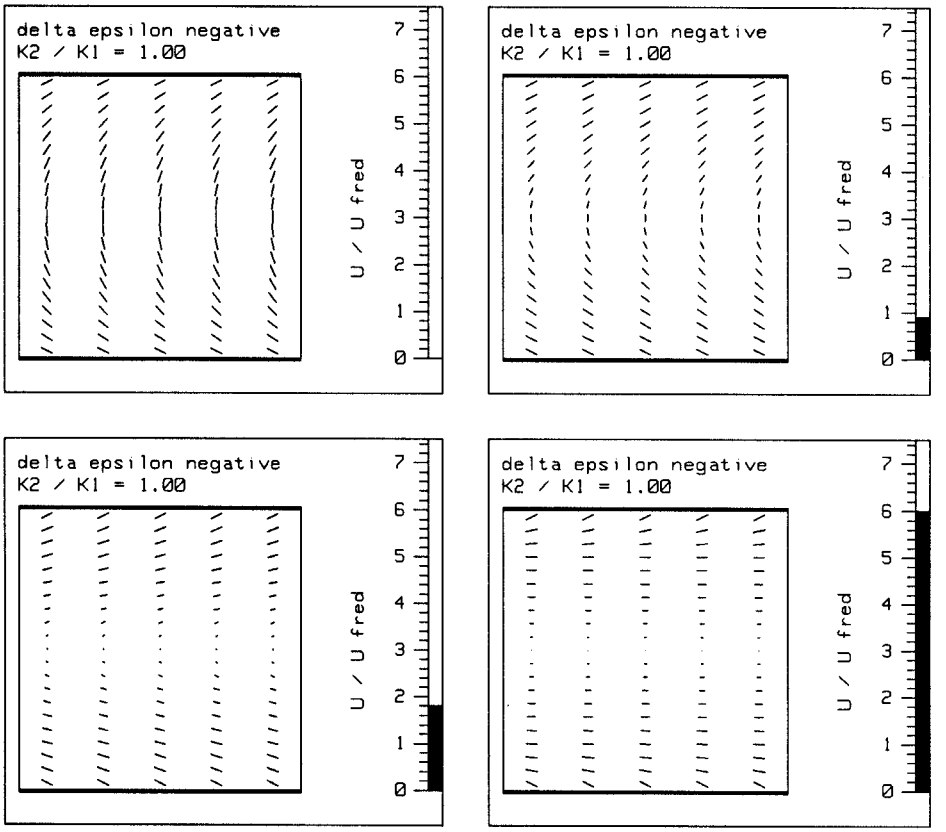

FIGURE 2 Director field of a π-cell with a negative dielectric anisotropy subjected to an electric field. Instead of switching to the H-state, the director field transforms continuously into an unstable twist state. When the electric field is turned off, the T-state decays back into the initial V-state.

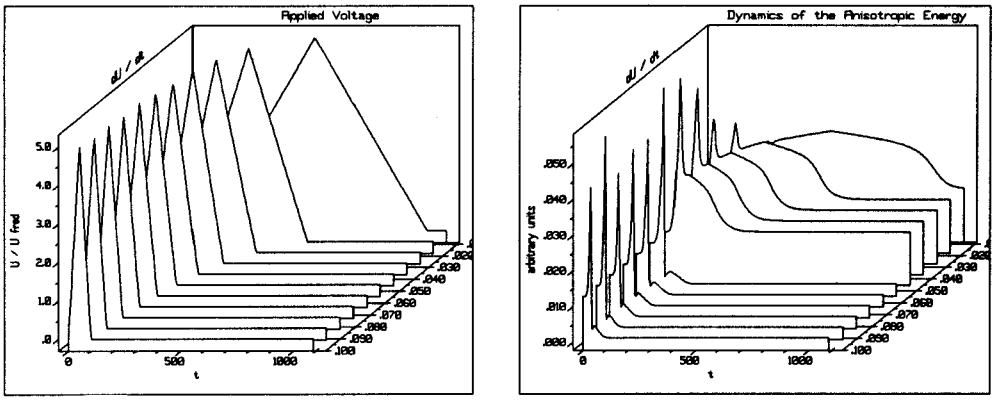

FIGURE 3 Time dependence of the anisotropic energies of a π-cell subjected to triangle-shaped pulses (left side) with a V-state as initial director configuration. Only for pulses with $dU/dt > 0.05$, the device switches to the H-mode, which can be recognized from the lower final energies.

applied pulse at a fixed ratio $K_2/K_1 = 0.8$, is exhibited as Figure 3. For a successful switching, the time for the pulse to reach its maximum value seems to be more important than its magnitude (which has to be above U_{fred}, of course). Secondly, the value of K_2 should be as small as possible (at least smaller than the other elastic coefficients). Finally, our simulations refer to a cell with absolutely no initial twist at the boundaries (a small twist angle of 1° makes the switching impossible).

CONCLUSIONS

The new tensorial algorithm can, in principle, simulate the observed phenomena, i.e. the H → V switching as well as the unsuccessful V → H switching. The π-cell, as a simple application is meant to demonstrate that the correct nematic symmetry is crucial not only for the occurrence of disclinations, but also for the transition between topological different configurations of the director field. This holds even even for a one-dimensional spatial dependence, where only disclination planes are possible.

In view of the application for device modeling, however, the algorithm should be considered only as a first step; the model used here can still be refined in several points:

1. Flow processes should be taken into account.
2. The restriction to the two-coefficient-approximation is, in principle, not necessary (see Equation (1–3)).
3. The one-dimensional spatial dependence, although widely used for cell ap-

plications, cannot describe disclinations. It would therefore be interesting, to examine the influence of the usual nematic defects on the cell operation.

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