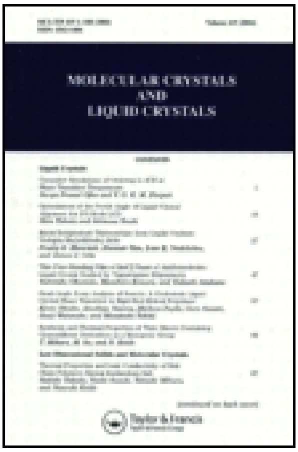

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Numerical Simulation of Director Distribution in Nematic Liquid Crystal Cells with Weak Anchoring Boundaries

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NUMERICAL SIMULATION OF DIRECTOR DISTRIBUTION IN NEMATIC LIQUID CRYSTAL CELLS WITH WEAK ANCHORING BOUNDARIES

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Abstract The general torque balance equations have been derived for the liquid crystal cells with weak anchoring boundaries by minimizing the bulk and surface free energy simultaneously [A. Sugimura, G. R. Luckhurst, and Z. Ou-Yang, Phys. Rev. E, 52, 681 (1995)]. The torque balance equations have been numerically solved to obtain the director distribution in the nematic liquid crystal cells with weak anchoring boundaries and the influence of the anchoring energy on the director distribution is elucidated.

INTRODUCTION

To describe the director distribution with weak anchoring surfaces for a homogeneous nematic liquid crystal (NLC) sample, Rapini and Papoular[1] (RP) have phenomenologically derived the anchoring energy per unit area which describes the anisotropic interaction between the nematic and the substrate,

$$g_s = -\frac{A}{2}(\underline{n} \cdot \underline{e})^2, \tag{1}$$

where $\underline{n}$ is the NLC director, $\underline{e}$ is the easy direction denoted by de Gennes[2], and A is the anchoring strength parameter which determines the ability of the director to deviate from the easy axis. On the basis of RP function, the influence of the director orientation in the NLC bulk has been studied in literature.[3–10] In these studies, RP energy in Equation (1) has been treated as a linear combination of the polar $g_s(\theta)$ and azimuthal $g_s(\phi)$ anchoring terms to simplify the mathematical analysis. However, there is no physical reason to do such separation and the surface energy density must be expressed as two-dimensional function $g_s(\theta, \phi)$.[11,12] Recently, we have derived the general torque balance equation by the variational method for the energy including both bulk and surface energies.

In this paper, we carry out the numerical calculation of the director distribution in NLC cells with weak anchoring boundaries using the general torque balance equations.

THEORY

We consider a nematic cell located between the two planes located at $X_3 = 0$ and $X_3 = L$, as illustrated schematically in Figure 1. The director $\underline{n}$ is expressed as ($\cos\theta\cos\phi$,$\cos\theta\sin\phi$,$\sin\theta$), where θ is the angle between the alignment layer surface and the director, and ϕ is the azimuthal angle of the director. In case of twisted chiral nematic (TCN) cell, the surface and bulk torque balance equations have been derived by minimizing the total free energy.[11,12] The surface torque balance equations at $X_3 = 0$ are written as

$$
\begin{aligned}
f(\theta)\theta^{(1)}|_{X_3=0} &= A(\sin\theta_o\sin\theta + \cos\theta_o\cos\theta\cos\phi) \\
&\quad \times(\cos\theta_o\sin\theta\cos\phi - \sin\theta_o\cos\theta), && (2) \\
h(\theta)\phi^{(1)}|_{X_3=0} &= -k_2\cos^2\theta \\
&\quad +A(\cos\theta_o\cos\theta\cos\phi + \sin\theta_o\sin\theta)\cos\theta_o\sin\phi\cos\theta, && (3) \\
f(\theta) &= k_{11}\cos^2\theta + k_{33}\sin^2\theta, \\
h(\theta) &= \cos^2\theta(k_{22}\cos^2\theta + k_{33}\sin^2\theta), && (4)
\end{aligned}
$$

where θ° is the orientation of the director at the nematic-wall interface, θ_o is the angle between the easy direction and the layer parallel, the constants k_{11}, k_{22} and k_{33} are the splay, twist, and bend elastic constants of the NLC, respectively, $\theta^{(1)} = d\theta/dX_3$, $\phi^{(1)} = d\phi/dX_3$, $k_2 = -2\pi k_{22}/p_o$, and p_o denotes the pitch of the material induced by a chiral dopant. The bulk torque balance equation is written as

$$
\begin{aligned}
f(\theta)\theta^{(2)} &+ \frac{1}{2}f_\theta\theta^{(1)2} - \frac{1}{2}h_\theta\phi^{(1)2} \\
&+ 2k_2\sin\theta\cos\theta\phi^{(1)} + \epsilon_o\Delta\epsilon E^2\sin\theta\cos\theta = 0, \qquad (5)
\end{aligned}
$$

$$
\phi^{(1)} = \frac{1}{h(\theta)}(C_1 - k_2\cos^2\theta), \qquad (6)
$$

where ϵ_o is the dielectric permittivity of vacuum, $\Delta\epsilon$ is the dielectric anisotropy in NLC, C_1 is a constant, $f_\theta = df/d\theta$, $h_\theta = dh/d\theta$, and $\theta^{(2)} = d\theta^{(1)}/dX_3$.

In case of the HN liquid crystal cell ($\phi = 0$, and $k_2 = 0$ for $p_o \to 0$), Equations.(2), (3), (5) and (6) are reduced to

$$f(\theta)\theta^{(1)}|_{X_3=0} = A(\sin\theta_o\sin\theta + \cos\theta_o\cos\theta)(\cos\theta_o\sin\theta - \sin\theta_o\cos\theta), \tag{7}$$

$$f(\theta)\theta^{(2)} + \frac{1}{2}f_\theta\theta^{(1)2} + \epsilon_o\Delta\epsilon E^2\sin\theta\cos\theta = 0. \tag{8}$$

From these two equations, we can obtain the director distribution, $\theta(X_3)$, in a HN slab at the steady state.

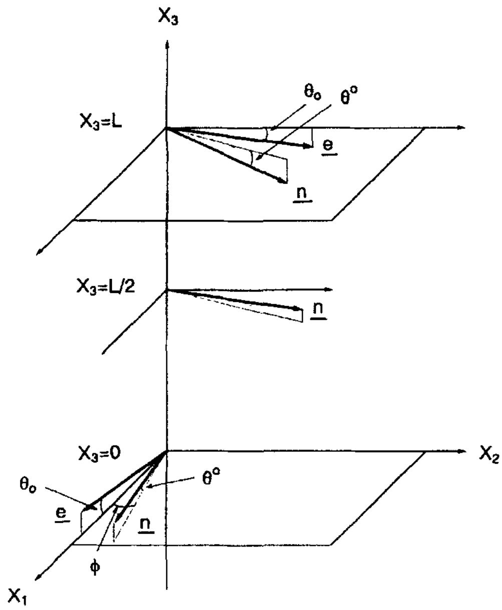

FIGURE 1 The geometry of the twisted chiral nematic cell located between the two planes $X_3 = 0$ and $X_3 = L$.

NUMERICAL PROCEDURE

The director distribution $\theta(X_3)$ and the electric field distribution are calculated at a number of points evenly distributed across the cell thickness, and separated from each other by a distance of ΔX_3. The calculation consists of the two steps. First, given $\theta(X_3)$, one calculates the corresponding electric field by using the Laplace equation with the successive over relaxation method. Second, given new electric field, one calculates the new director distribution to satisfy the boundary condition, $\theta(0) = \theta(L)$ (an antiparallel cell) or $\theta(0) = -\theta(L)$ (a parallel cell), with the Runge-Kutta method. Physical quantities used in the numerical calculation were $L = 5.8$ μm, $k_{11} = k_{33} = 11.8 \times 10^{-12}$ N, $\theta_o = 6.0°$ and $\Delta\epsilon = 9.9$, respectively.

RESULTS AND DISCUSSION

We first examine the influence of $\theta°$ at the nematic-wall interface on the anchoring strength parameter for both parallel and antiparallel NLC cells. The results are shown in Figure 2. For an antiparallel cell $\theta°$ is independent of A, whereas for a parallel cell $\theta°$ decreases from 6° to $\sim$ 0° with decreasing A. Such decrease is due to the fact that the orientation of the director in the NLC bulk influences that at the nematic-wall interface in case of weak anchoring energy.

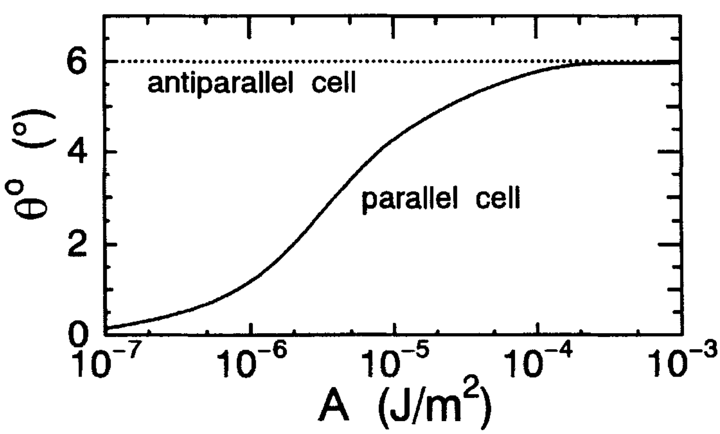

FIGURE 2 Dependence of $\theta°$ on the anchoring strength parameter A in the absence of applied voltage for antiparallel and parallel NLC cells.

Next, we examine the effect of electric field application to the antiparallel NLC cell with weak anchoring boundaries. Figure 3 shows $\theta°$ at the nematic-wall interface at various applied voltages for the NLC cells with different anchoring energy. With increasing applied voltage, the orientation of the director at the interface becomes homeotropic for weak anchoring boundaries but is almost constant for strong anchoring boundaries. It is obvious that the anchoring energy also play a key role for the control of the orientation of the director at the nematic-wall interface under the voltage application.

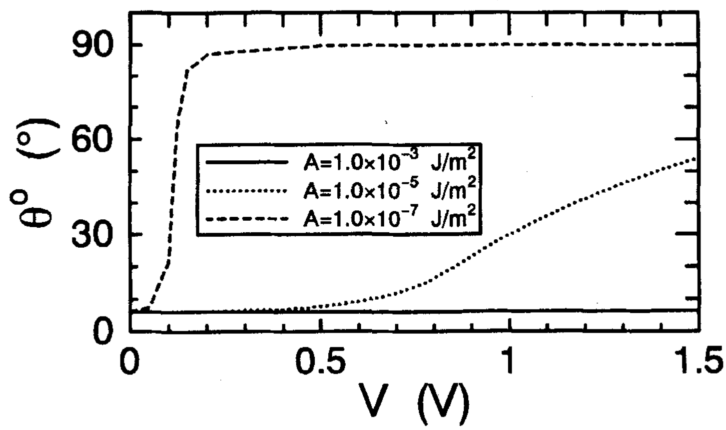

FIGURE 3 A plot of θ° vs V for three different anchoring energies.

We show in Figure 4 the director distribution in the NLC slab at 1.5 V for three different anchoring energies. In case of weak anchoring energy, the director homeotropically aligns in the direction of the applied electric field. As the anchoring energy is increased, we see in Figure 4 that $\theta(X_3)$ has the maximum value at $X_3 = L/2$ and the values of $\theta(X_3)$ is decreased in the NLC slab. We note here that the director distribution under the application of electric field can be modified by the anchoring energy.

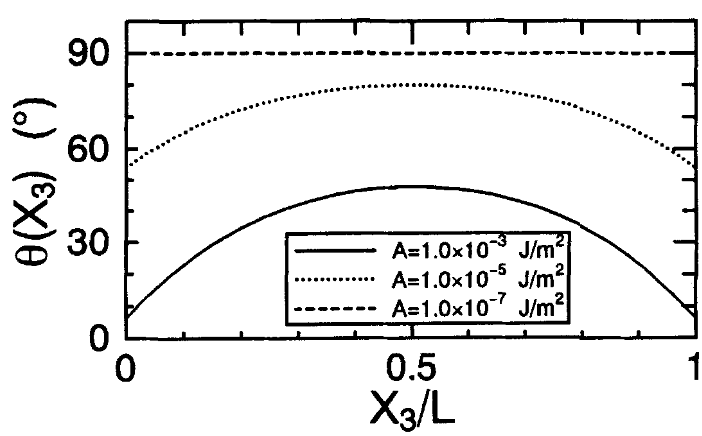

FIGURE 4 Director distribution at the applied voltage of 1.5 V for three different anchoring energies.

CONCLUSIONS

We have numerically analyzed the torque balance equation for homogeneous NLC cells to examine the influence of weak anchoring boundaries. It is found that the dependence of the orientation of the director at the nematic-wall interface on the anchoring energy for a parallel homogeneous NLC cell is totally different from that for an antiparallel homogeneous NLC cell. It is also found that for an antiparallel homogeneous NLC cell the director distribution under the application of electric field is significantly altered by the anchoring energy strength. These characteristics of weak anchoring boundaries would be useful for a novel NLC display.

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