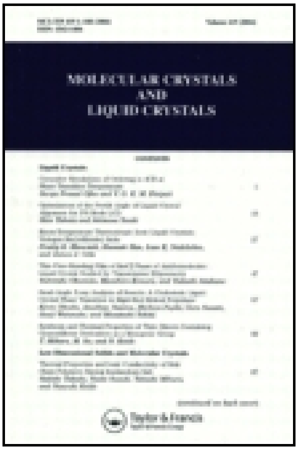

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Director Reorientation in a Cell with Time-Dependent Anchoring Due To Adsorption/ Desorption of LC Molecules

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DIRECTOR REORIENTATION IN A CELL WITH TIME-DEPENDENT ANCHORING DUE TO ADSORPTION/DESORPTION OF LC MOLECULES

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The time evolution of the director orientation in a nematic cell due to the adsorption/desorption processes of LC molecules on the cell substrate is considered. It is shown that boundary conditions on the cell surface evolve in accordance with the orientation distribution function of LC molecules in the cell bulk. During the time evolution the orientational distribution function of molecules adsorbed on the cell substrate possesses two maximums. Switching off the magnetic field at the suitable moment one can obtain a bistable nematic system.

Keywords: anchoring energy; liquid crystals; memory-free alignment

1. INTRODUCTION

The possibility to control precisely the anchoring energy of liquid crystals (LC) on photo aligning polymers makes them the most promising materials for weak and memory-free anchoring. The problem, which hampers their application, is the strong alignment memory effect. This effect is caused by an anisotropic adsorption of LC molecules on aligning surface and is observed for most aligning materials and different liquid crystals [1–8]. The adsorbed layer behaves as a new anisotropic substrate, imposing strong monostable anchoring [2]. The strength of anchoring depends on

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the number of adsorbed LC molecules and their orientational distribution function. The memory alignment can be changed due to adsorption and desorption of LC molecules.

The purpose of the present paper is to investigate the time evolution of the director orientation in the cell subject to external magnetic (or electric) field in the case of time-dependent boundary conditions determined by the processes of adsorption/desorption of LC molecules on the cell substrate.

2. EQUATION FOR DIRECTOR ORIENTATION

Let us consider a nematic cell bounded by the planes $z = 0$ and $z = l$. We suppose the director anchoring at the plane $z = 0$ to be planar and infinitely strong, with the director easy axis along the axis Ox. The director anchoring at the plane $z = l$ is planar as well but both the director easy axis and anchoring energy depend on the adsorption/desorption processes of LC molecules on this plane. At $t = 0$ the magnetic field $\vec{H} = H\vec{e}_y$ is switched on ($\vec{e}_y$ is a unit vector along the axis Oy, see Fig. 1). Then the director orientation in the cell bulk changes that has an effect on the adsorption/desorption processes of LC molecules on the plane $z = l$. As a result the boundary conditions on the plane $z = l$ change as well and influence (in their turn) the director orientation in the cell bulk. We suppose the director orientation in the cell bulk to follow adiabatically the boundary conditions.

Denoting the director angle with the axis Ox by φ one can seek the director spatial distribution in the form

$$\vec{n}(z) = \vec{e}_x \cos\varphi(z) + \vec{e}_y \sin\varphi(z) \tag{1}$$

Using this notation we can write the expression for nematic cell free energy in the magnetic field

$$F = \frac{1}{2}\int_0^l dz \left[K\left(\frac{\partial\varphi(z,t)}{\partial z}\right)^2 - \chi_a H^2 \sin^2\varphi(z,t)\right] - W_S(t)$$

(here we use one constant approximation) and taking the variation of this functional we obtain the equation

$$\varphi''(z) + \frac{\chi_a H^2}{K}\sin\varphi(z)\cos\varphi(z) = 0, \quad 1/\xi^2 = \chi_a H^2/K \tag{2}$$

with boundary conditions

$$\varphi(0) = 0, \quad \left[K\varphi'(z) - \frac{\partial W_S[\varphi(z)]}{\partial\varphi(z)}\right]_{z=l} = 0 \tag{3}$$

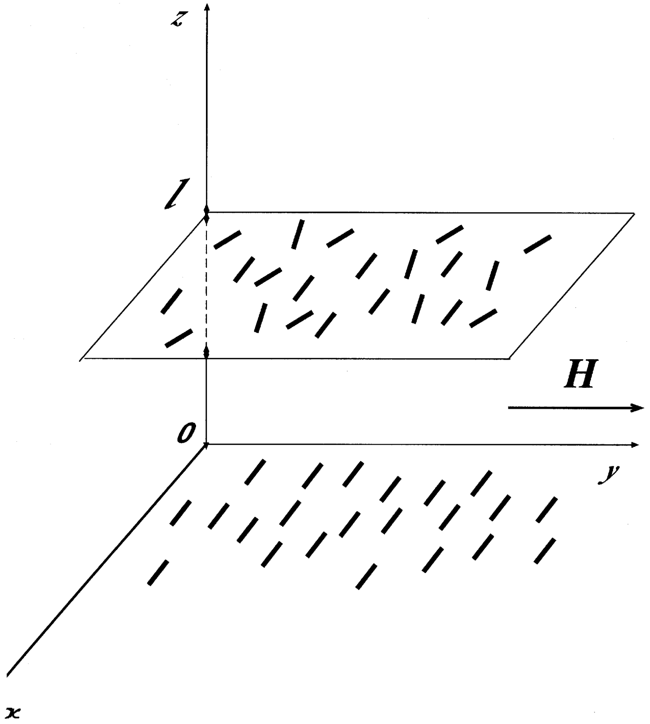

FIGURE 1 Schematic representation of the nematic cell.

Here K is the Frank's elastic constant, χ_a is the magnetic susceptibility anisotropy, $W_S(\varphi)$ is the director anchoring energy at the plane $z = l$ whose real form depends on the adsorption/desorption processes and has to be defined afterwards.

One can write the solution of the Eq. (2) in the form

$$\sin\varphi(z) = k\,\mathrm{sn}(z/\xi, k) \tag{4}$$

were $\mathrm{sn}(\alpha z, k)$ is an elliptic Jacobi sine function, the parameter k can be determined from the second boundary condition (3) which takes the form

$$\left[\frac{k}{\xi}\mathrm{cn}(\varphi(z), k) - \frac{1}{K}\frac{\partial W_S[\varphi(z)]}{\partial\varphi(z)}\right]_{z=l} = 0. \tag{5}$$

Thus, the director distribution in a nematic cell is described by the expressions (4) and (5). To calculate it we have to know the true form of the director anchoring energy $W_S[\varphi]$.

3. ANCHORING ENERGY AND BOUNDARY CONDITIONS

We suppose the interaction of LC molecules with molecules of the substrate material to be isotropic one and the only interaction with adsorbed on the substrate LC molecules gives the contribution to the anchoring energy $W_S[\varphi]$. Similarly to Mayer-Saupe theory [4] one can introduce the orientation distribution function for LC molecules near the cell surface

$$f_{vol}(\boldsymbol{\Omega}_1, t) = \frac{1}{N_{vol}} \exp\Big(\beta P_2(\vec{l}_1 \cdot \vec{n})\Big), \quad \beta = \frac{aS}{k_B T}, \tag{6}$$

where

$$\vec{l}_1 = (\sin\theta_1 \cos\varphi_1, \sin\theta_1 \sin\varphi_1, \cos\theta_1) \tag{7}$$

is a unit vector along the long molecule axis, P_2 is a Legendre polynomial, S is the order parameter, a is a constant that describes the strength of molecular anisotropic interaction in the mean field approximation, $\boldsymbol{\Omega}_1 = \{\theta_1, \varphi_1\}$, and N_{vol} is a normalization constant. Here the director $\vec{n}$ depends on the time due to adsorption/desorption processes on the plane $z = l$.

We denote the orientation distribution function of the molecules adsorbed on the cell substrate by $f_{surf}(\boldsymbol{\Omega}_2, t)$. It is evident that

$$f_{surf}(\boldsymbol{\Omega}_2, t) = f_S(\varphi_2, t)\delta(\cos\theta_2) \tag{8}$$

where the last multiplier displays the fact that all the molecules lie on the substrate.

Further we adopt that interaction between LC molecules and molecules in the bulk near the surface depends on their long axes orientation in the form $(\vec{e}_1 \cdot \vec{e}_2)^2$, where $\vec{e}_{1,2}$ are the unit vectors along the long axis of molecules. Hence we assume the following expression for $W_S[\varphi]$:

$$W_S[\varphi] = W_0 \iint d\boldsymbol{\Omega}_1 d\boldsymbol{\Omega}_2 (\vec{l}_1 \cdot \vec{l}_2) f_{vol}(\boldsymbol{\Omega}_1, t) f_{surf}(\boldsymbol{\Omega}_2, t), \quad W_0 < 0 \tag{9}$$

where $\vec{l}_2$ is a unit vector along the long axis of the adsorbed molecule.

Substituting the expressions (6), (8) into (9) we arrive to the following expression for the director anchoring energy

$$W_S[\varphi] = \frac{1}{2}\left[I_S(t)\bar{I}_V(t) + \bar{C}_{2V}(t)\sqrt{C_{2S}^2(t) + S_{2S}^2(t)} \cos 2(\varphi - \varphi_S(t))\right] \tag{10}$$

where the angle $\varphi_S(t)$ is defined as

$$\sin 2\varphi_S(t) = \frac{S_{2S}(t)}{\sqrt{C_{2S}^2(t) + S_{2S}^2(t)}}, \quad \cos 2\varphi_S(t) = \frac{C_{2S}(t)}{\sqrt{C_{2S}^2(t) + S_{2S}^2(t)}} \tag{11}$$

and

$$
\begin{aligned}
&I_S(t) = \int_{-\pi/2}^{\pi/2} f_S(\alpha,t)\,d\alpha, \quad \bar{I}_V(t) = \int_{-\pi/2}^{\pi/2} \bar{f}_V(\alpha,t)\,d\alpha,\\
&\bar{C}_{2V}(t) = \int_{-\pi/2}^{\pi/2} \bar{f}_V(\alpha,t)\cos 2\alpha\,d\alpha, \quad \bar{f}_V(\varphi_1,t) = \int_0^{\pi} f_{vol}(\mathbf{\Omega}_1,t)\sin^3\alpha\,d\alpha \qquad (12)\\
&C_{2S}(t) = \int_{-\pi/2}^{\pi/2} f_S(\alpha,t)\cos 2\alpha\,d\alpha, \quad S_{2S}(t) = \int_{-\pi/2}^{\pi/2} f_S(\alpha,t)\sin 2\alpha\,d\alpha
\end{aligned}
$$

The expression (10) is similar to Rapini potential [3] but the strength of anchoring and the easy axis orientation are now time dependent.

Since the distribution function $f_{vol}(\mathbf{\Omega}_1,t)$ is supposed to be known (see Eq. (6)) we can calculate $\bar{I}_V$ and $\bar{C}_{2V}$. But to find I_S, C_{2S} and S_{2S} we need to know the distribution function $f_S(\varphi,t)$ for molecules on the cell substrate.

One can write the following kinetic equation:

$$\frac{\partial f_S(\varphi_1,t)}{\partial t} = A_+ f_V(\varphi_1,t) - A_- f_S(\varphi_1,t) \qquad (13)$$

where $f_V(\varphi_1,t) = \int_0^{\pi} f_{vol}(\mathbf{\Omega}_1,t)\sin\theta_1 d\theta_1$ is a 2-dimensional projection of the function (6), $A_\pm$ are the coefficients describing the velocities of the adsorption/desorbtion processes. As an initial condition for the Eq. (13) we choose its stationary form:

$$f_S(\varphi_1,0) = \frac{A_+}{A_-} f_V(\varphi_1,0) \qquad (14)$$

If the distributions $f_S(\varphi,t)$ and $f_V(\varphi,t)$ are normalized, the kinetic equation must be changed in order to meet the requirement (14). It occurs that it is sufficient to put $A_+ = A_-$ in this case. To find C_{2S} and S_{2S} we can multiply both sides of the Eq. (13) for the first by $\sin 2\varphi_1$ and for the second by $\cos 2\varphi_1$. Then, upon integrating obtained expressions over φ_1 and t we get:

$$
\begin{aligned}
S_{2S}(t) &= S_{2S}(0)e^{-A_- t} + A_+ C_{2V} \int_0^t e^{-A_+(t-\tau)} \sin 2\varphi(t) d\tau\\
C_{2S}(t) &= C_{2S}(0)e^{-A_- t} + A_+ C_{2V} \int_0^t e^{-A_+(t-\tau)} \cos 2\varphi(t) d\tau
\end{aligned} \qquad (15)
$$

where

$$C_{2V} = \frac{2}{N_{vol}} \frac{\pi e^{-\beta/2}}{3\beta/2} \left(e^{3\beta/2} - 1 \right) - 1 \tag{16}$$

Similarly, integrating the Eq. (13) over φ_1 and t we obtain

$$I_S(t) = A_+/A_- \tag{17}$$

(is constant). Using the expressions (12), (15), (17) into the formula (10) we arrive to the following form of the boundary condition (5):

$$\left[\alpha k \operatorname{cn}(z/\xi, k) + W_0[S_{2S}(0)\cos 2\varphi - C_{2S}(0)\sin 2\varphi] e^{-A_- t} - W_0 C_{2V}(t)\bar{C}_{2V}(t) \int_0^t e^{-A_-(t-\tau)} \sin 2(\varphi - \varphi(\tau)) d\tau \right]_{z=l} = 0 \tag{18}$$

where $\bar{C}_{2V}(t)$ and $C_{2V}(t)$ are determined by the formulas (12), (16) and $C_{2S}(0)$ and $S_{2S}(0)$ can be easily calculated using the condition (14). Finally, it should be noted here that both the angle φ and parameter k in equations (4), (18) depends now on the time t.

5. NUMERICAL CALCULATIONS AND RESULTS

The Eqs. (4), (18) as well as the Eq. (13) were solved numerically at the next values of parameters: $\frac{W_0 \xi}{K} = 10^{-2}$, $\frac{l}{\xi} = 2$ and $A_+ = A_- = 1\,s^{-1}$, if $l = 100\,\mu$, the value of magnetic field is $H = 200\,\text{Gs}$. Some results of the calculations are presented on Figures 2–4. The solution of the differential equation was developed with the use of standard Runge-Kutta method, and at each step of this procedure we solve the algebraic equation to find the parameter k of the elliptic functions.

On Figure 2 the time evolution of orientation distribution function $f_S(\varphi, t)$ of molecules adsorbed on the cell substrate is shown. One can see that after the magnetic field is switched on the distribution function $f_S(\varphi, t)$ changes forced by the adsorption on the cell substrate of LC molecules from the cell bulk with orientation distribution described near the cell plane $z = l$ by the function $f_V(\varphi(z = l), t)$. It is interesting to note that during the time evolution the function $f_S(\varphi, t)$ can possess two maximums. It means that if at the proper moment the magnetic field is switched off one can obtain a bistable nematic system.

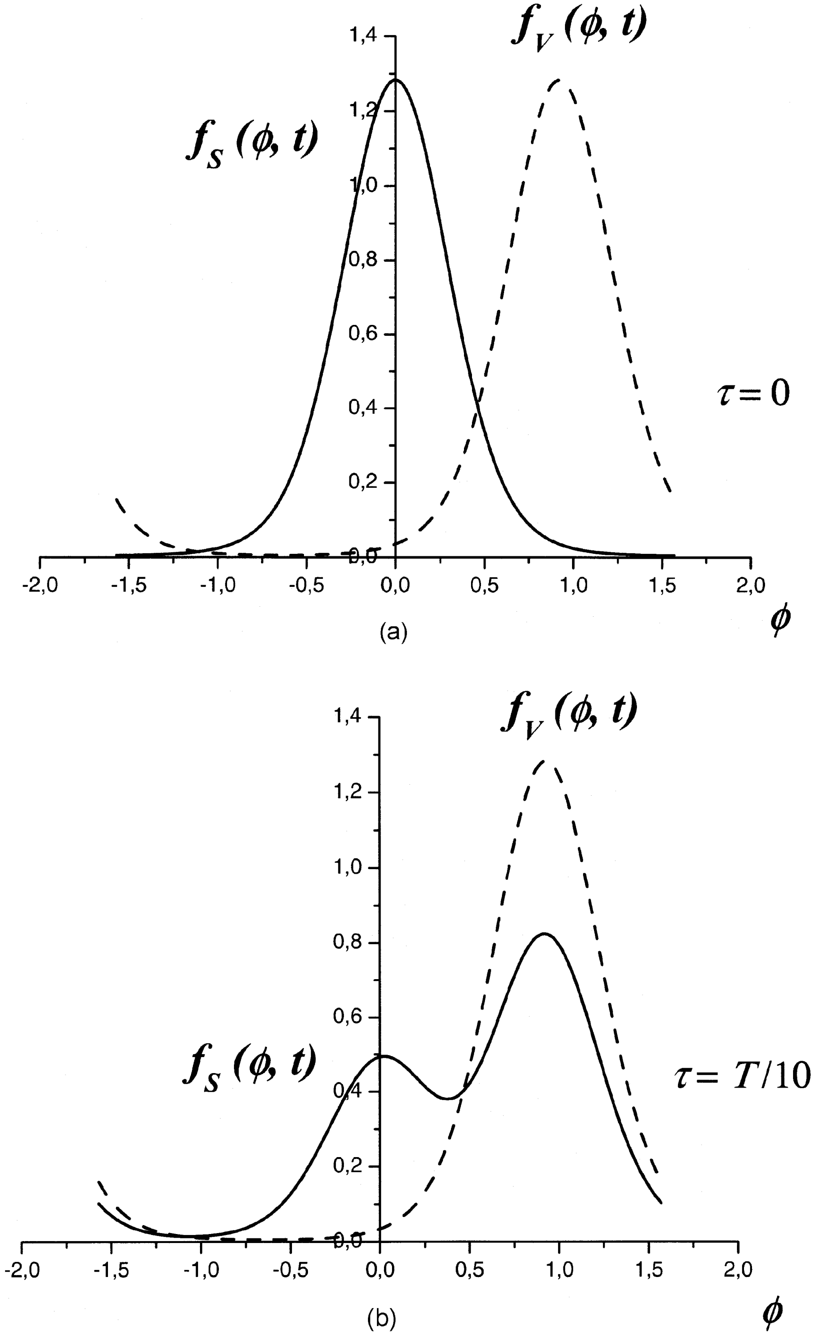

FIGURE 2 Distribution functions for different time moments: a)$\tau = 0$, b)$\tau = T/10$, c)$\tau = T/5$, d)$\tau = T$, where $T = 10$, $\tau = A_{-}t$.

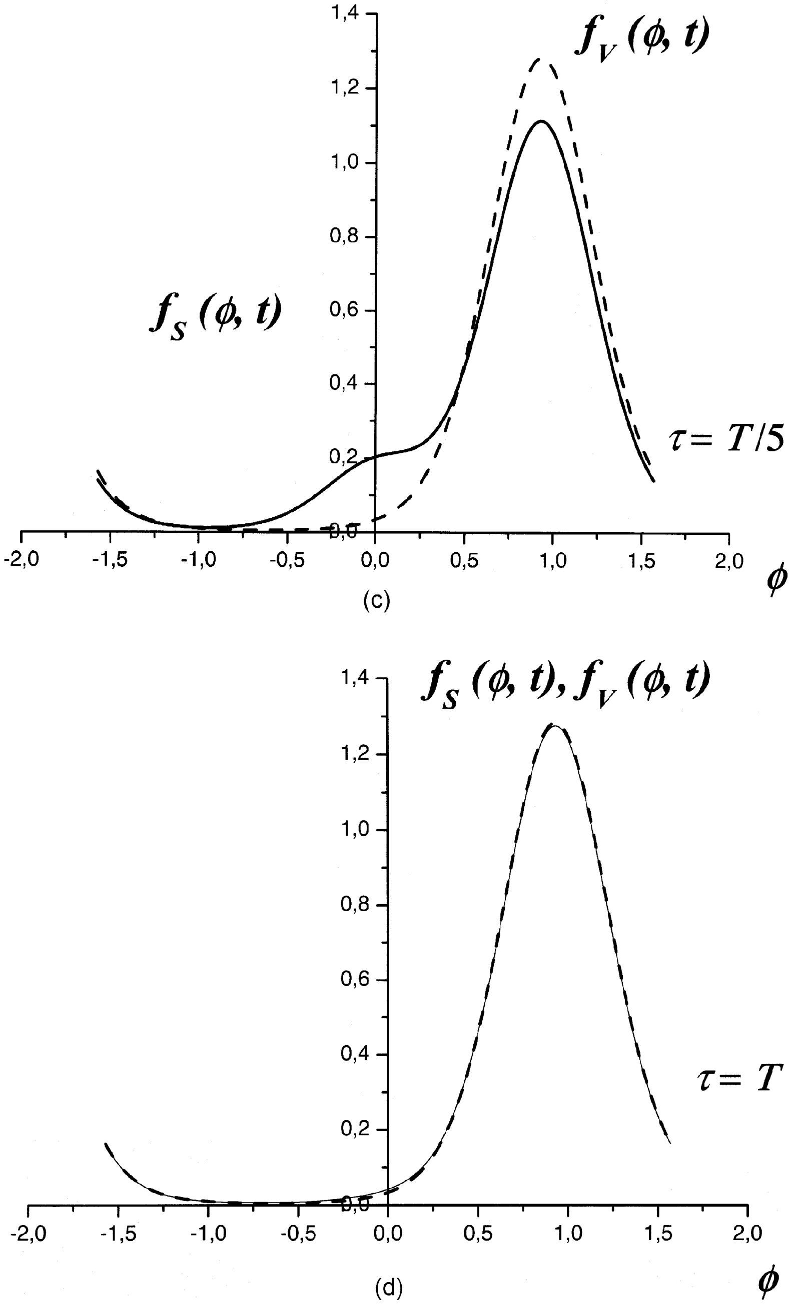

FIGURE 2 Continued.

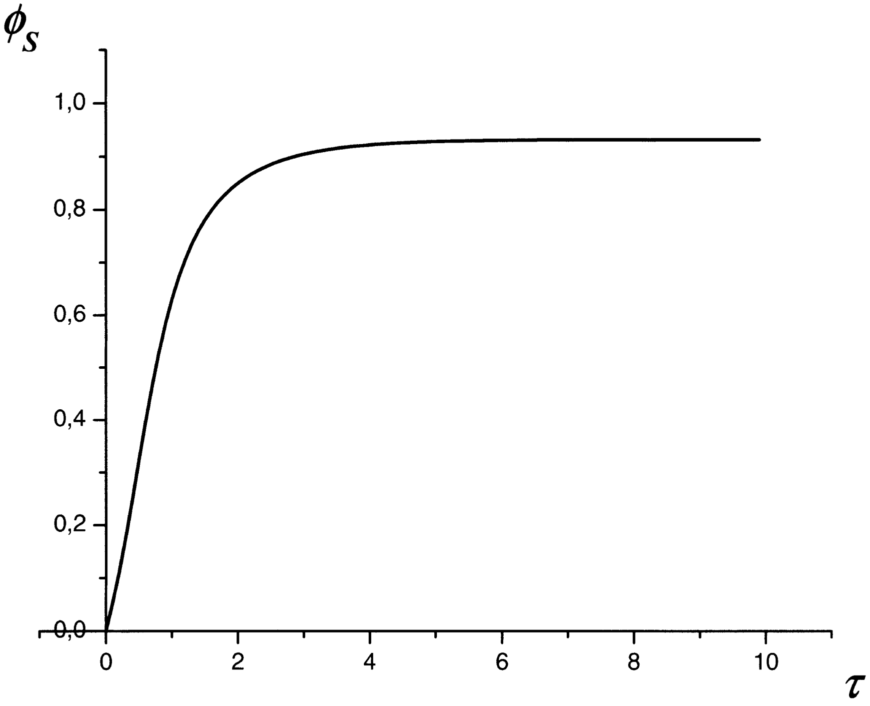

FIGURE 3 Time evolution of $\varphi(z,t)$, here $\tau = A_{-}t$ and $z = l$.

The time evolution of the director orientation near the cell plane $z = l$ due to the adsorption/desorption processes of LC molecules is shown on Figure 3. Figure 4 presents the change with time of the angle φ_S, which describes "the easy axis" direction in the Rapini-Papoular-like formula (10). As we can see from the Figures 3 and 4, when the strength of the magnetic field is sufficiently large, the value of the volume angle $\varphi(l,t)$ near the surface at $t = 0$ approximately equals to its asymptotic value at $t = \infty$. This situation is precisely described by the solution with the parameters we have chosen.

It occurs that the angles φ_S and $\varphi(l,t)$ runs to the same limit when $t \to \infty$ which is different from the case when adsorption/desorption process is absent.

Finally we note that the adsorption/desorption processes of LC molecules can essentially influence on the boundary conditions on the cell surface. This effect can be used to obtain a bistable nematic system. We mean that when the magnetic field is turned off at the suitable moment of time (see Fig. 2) the distribution function at the surface have two

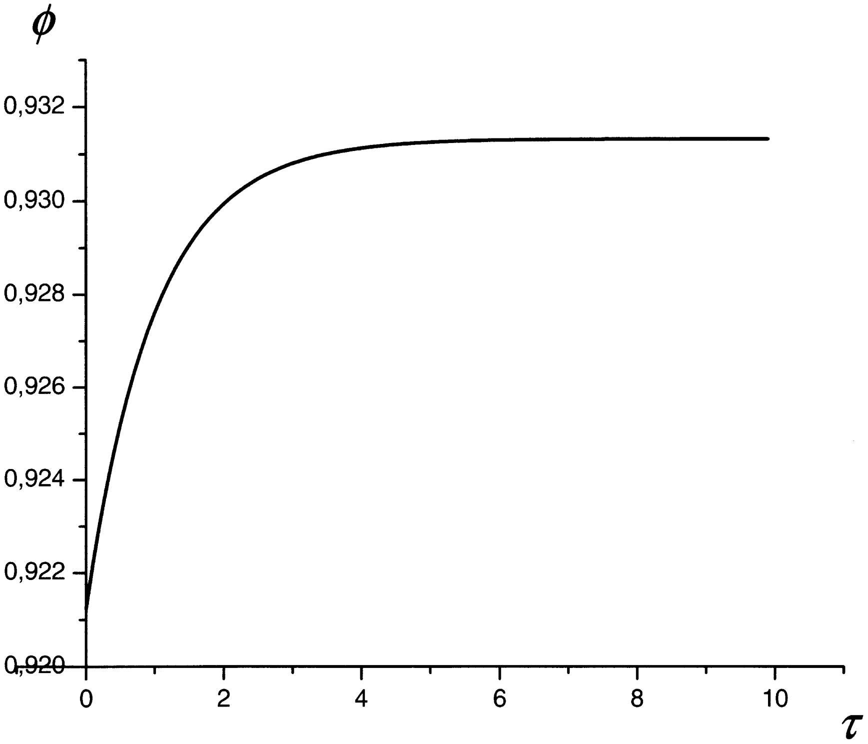

FIGURE 4 Time evolution of $\varphi(z,t)$, here $\tau = A_{-}t$.

maxima. Of course, the process will be reversed in this case and the system returns to initial conditions at $t = 0$.

6. SUMMARY

In the present paper we have considered the time evolution of the director orientation in a nematic cell due to the adsorption/desorption processes of LC molecules on the cell substrate.

The adsorption/desorption process is described by the kinetic equation and the model for anchoring energy (Rapini-like energy). It is shown that boundary conditions on the cell surface evolve in accordance with the orientation distribution function of LC molecules in the cell bulk. Numerical calculations show that during the time evolution the orientational distribution function of molecules adsorbed on the cell substrate possesses two maximums. Switching off the magnetic field at the suitable moment one can obtain a bistable nematic system.

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