Simulation of frequency dependence of dielectric susceptibility for description of director reorientation dynamics of nematic LC

Vakulin D.A., Ivanov A.V.
ITMO University, Kronverkskii pr. 49A, 197101, Saint Petersburg, Russia
vakulin.dmitry@gmail.com

Abstract. Simulation of the liquid crystal behavior in an external electric field allows to determine the characteristics of the LC device for specific control signal. The reorientation of director tilt angles is described by the Frank-Oseen elasticity theory, by the Leslie-Ericksen hydrodynamics theory and also by Maxwell system of electromagnetic equations. Due to the fact that it is difficult to obtain analytical solution of dependencies polar and azimuthal angles on time it is necessary to use numerical methods. The numerical solution allows to determine the characteristics of the LC device for specific control signal, but it does not allow to solve the inverse problem. It is determining the necessary parameters of the control signal. To solve this problem, we obtained an approximate analytical solution of the dynamics equations of the director reorientation under the electric field for arbitrary values of the elastic constants and boundary conditions. The results of numerical simulation of the director reorientation under the electric field in hybrid-oriented structure of a dual-frequency nematic liquid crystal were obtained. It is shown that results of analytical solution are in good agreement with the results of computer simulation and experiment in case of small deformations of the LC layer and used approximations.

1. Introduction
Widespread use of nematic liquid crystals (NLC) in the optical components of high-speed telecommunication systems due to the presence of specific properties of these materials: stability, fast response, low loss operation over a wide temperature range management via low voltage, low power consumption. With LC technology to produce fiber-optic systems, optical switches, modulators, filters, attenuators, equalizers, polarization controllers and other devices.

One of the important characteristics of the electrically controlled optical elements based on the LC that affect the performance of telecommunication networks is the time to switch between operating states. To speed up the switch to LC devices use hybrid-oriented (HAN - hybrid aligned nematic) cell with a dual frequency (DF) NLC [1, 2]. Have DF addressing HAN devices allows you to control the process of switching from the «OFF» → «ON» → «OFF» by changing the frequency applied to the cell of an external electric signal.

Changes angles director of NLC by an electric field described by the theory of elasticity Franca Oseen [3,4], the theory of hydrodynamic Leslie-Ericksen for nematic phase [5], as well as the system of Maxwell's electromagnetic equations. Given the complexity of the resulting system of equations to determine the spatial and temporal dependence of the polar and azimuthal angles of the NLC director usually use numerical methods [6-8]. The numerical calculation allows you to get listed
according to the given parameters of the control signal: field strength, frequency, pulse duration and shape. However, the simulation LC devices often need to solve the inverse problem - to define the parameters of the control signal to produce a predetermined angle distribution director. To achieve this goal it is necessary to find an analytical solution of the equations describing the dynamics of the director reorientation that can only be done using some approximations.

The purpose of this paper is to obtain approximate analytical solutions of equations describing the dynamics of the reorientation of the molecules in the NLC DF HAN structure under the influence of an electric signal of arbitrary shape for modeling the optical response.

2. Simulation optical response

2.1. Equations of dynamics

A characteristic feature is the presence of DF NLC frequency dispersion of the dielectric constant. The values of the components of the dielectric constant of the NLC electronic transitions are determined by the external field and the corresponding polarizabilities. LC full polarization of the medium can be represented as the sum of the contributions of the electronic polarization of individual atoms and molecules and the orientation of the polarization of permanent molecular dipoles $P = P_e + P_o$. The anisotropy of the NLC molecules is determined by various polarizability with respect to the molecular axis (the director), hence the need to introduce as the sum of the polarization parallel and perpendicular to the axis of the component $P = P\parallel + P\perp$.

As in the present study carried out modeling of the optical response of the NLC to the millisecond time range, used for the theoretical description of the Debye model of dielectric relaxation. In this model it is assumed that the forced response of the orientation of the polarization component parallel to the director obeys Langevin type [7]:

$$\tau \frac{dP^o_\parallel}{dt} + P^o_\parallel = \alpha E_\parallel,$$

(1)

We write the equations for calculating the dynamics of change in the angle of inclination of the director in the structure of the HAN in the approximation when the moment of inertia of the molecules and streaming effects can be neglected. Then we obtain the following system of equations:

$$\gamma_1 \frac{\partial \theta_{z,t}}{\partial t} = (K_{33} - K_{11}) \sin \theta_{z,t} \cos \theta_{z,t} \left( \frac{\partial \theta_{z,t}}{\partial z} \right)^2 + f_{z,t} \frac{\partial^2 \theta_{z,t}}{\partial z^2} + P^e_{z,t} E_{z,t},$$

(2)

$$\tau \frac{dP^o_\parallel}{dt} + P^o_\parallel = \chi^{\circ}_e \varepsilon_0 E_{z,t} \sin \theta_{z,t}, \quad f_{z,t} = K_{11} \cos^2 \theta_{z,t} + K_{33} \sin^2 \theta_{z,t},$$

$$P^e_{z,t} = (P^o_{z,t} + P^o_{\perp}) \cos \theta_{z,t} \pm (P^o_{z,t} + P^o_{\perp}) \sin \theta_{z,t},$$

$$P_{\parallel}^e = \chi^{\circ}_e \varepsilon_0 E_{z,t} \cos \theta_{z,t}, \quad P_e = \chi^{\circ}_e \varepsilon_0 E_{z,t} \sin \theta_{z,t},$$

$$E_{z,t} = \frac{V_t}{d_0} - \frac{P^t_{z,t}}{\varepsilon_0} + \frac{1}{d_0 \varepsilon_0} \int_0^d P^e_{z,t} dz,$$

(3)

(4)

where $\gamma_1$ - rotational viscosity LC, $\varepsilon_0$ - dielectric constant, $K_{11}$ and $K_{33}$ - elastic coefficients Frank, $\chi^{\circ}_i$ - electronic (orientation) dielectric susceptibility for the $i$-component of polarization, $\chi^{\circ}_0$ - orientation dielectric susceptibility in the low-frequency limit, $V_t$ - potential difference between two electrodes, $d_0$ - the thickness of the LC layer. The expression for the electric field in the $z$ direction obtained by the Maxwell equations. To describe the dynamics of the director reorientation under the
influence of the electric field required to find a self-consistent solution of the above recorded for initial angles director. The system of equations (2) - (4) and a numerical method of its calculation model polar structure of DF bistable nematic liquid crystal has been proposed in [7], and the computer simulation of the dynamics of the director reorientation for a more general case of a twist structure is made in [8].

2.2. Approximate analytic solution

As previously noted, the analytical solutions for the resulting system of equations is required to use additional approximation [8, 9]. So in the case of large amplitude of the control voltage can be assumed that the forces caused by an external electric field is much larger than the effect of the elastic forces, and neglect terms depending on the elasticity coefficients Frank. We make one more assumption, often used when considering the impact of a control signal to the liquid crystal layer, we assume that the electric field in the LC layer is constant and equal to

\[ E_{\text{t}} = \frac{V_{\text{t}}}{d_0} \] [10]. Then, equations (2) - (4), which will now determine the change in tilt of the director in time to a certain point \( z_0 \), takes the following form:

\[ \frac{\partial \theta_{||,t}}{\partial t} = \varepsilon_0 \Delta \chi \sin \phi \cos \theta_{||,t} + P_{||,t} \cos \theta_{||,t}, \]

\[ \frac{dP_{||,t}}{dt} = \varepsilon_0 \Delta \chi \sin \phi \cos \theta_{||,t} + \Delta \chi = \chi^e - \chi^e - \chi^e. \] (5)

By setting the initial spatial distribution of the director tilt LC layer thickness and calculating the time dependence for each point of this distribution, you can get a full dependence \( \theta_{||,z,t} \).

Consider the dynamics of the director reorientation in time under the influence of the periodic electrical signal of arbitrary shape, presenting it as a Fourier series:

\[ V_i = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[ a_n \cos(nft) + b_n \sin(nft) \right], \] (6)

where \( f \) - frequency electric field, \( a_n \) and \( b_n \) - Fourier coefficients. A solution of the equations for the director parallel component orientation polarization \( P_{||} \) will be sought in the form of a product of two functions - a slowly varying amplitude \( \chi(t) \) and a periodic function with the period of the external field \( g(t) \):

\[ P_{||} = \chi(t) g(t), \quad g(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[ a_n \cos(nft) + b_n \sin(nft) \right]. \] (7)

Periodic function \( g(t) \) in (7) is represented as a Fourier series with coefficients \( a_n \) and \( b_n \). Using approximate equation for the derivative with respect to time \( P' = \chi' g + \chi g' \approx \chi g' \) in the case of the slowly varying amplitude, the second equation (5) can be rewritten as follows:

\[ \tau \frac{dg(t)}{dt} + g(t) = \frac{\varepsilon_0 \Delta \chi_{||}}{d_0} \sin \theta(t) V(t) \frac{\chi(t)}{\chi(t)}. \] (8)

Further, in the equation (8) perform the replacement of periodic functions of their Fourier series (6) and (7) and express the expansion coefficients \( a_n \) and \( b_n \) of the coefficients \( a_n \) and \( b_n \). Then the expression (7) for the orientation of the polarization \( P_{||} \) takes the following form:

\[ P_{||} = \frac{\varepsilon_0 \Delta \chi_{||}}{d_0} \sin \theta(t) P(t), \quad P(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[ a_n \frac{-nf \tau \phi}{1 + (nf \tau)^2} \cos(nft) + \frac{b_n + nf \tau a_n}{1 + (nf \tau)^2} \sin(nft) \right]. \] (9)
Substituting (9) in the first equation (5) which will carry out the separation of variables in the differential equation and find a solution to the director tilt. Finally, we obtain the expression

\[
\ln tg \theta_1 \bigg|_{t_0}^{t_f} = \frac{\varepsilon_0}{\gamma_1 d_0^2} \bigg( \Delta \mathcal{X} \int_0^{t_f} V^2(t) dt + \chi^{\circ} \int_0^{t_f} P(t) V(t) dt \bigg),
\]

(10)

where \( \theta_1 \) - the initial value of the angle of the director and the integrands Expressions containing Fourier series (6) and (9) that can be easily integrated (due to the bulkiness of these expressions, they write in this paper not shown). Equation (10) can be used to determine the time dependence of the tilt of the director, and for determining the parameters of the control signal under the influence of which the angle will move to a predetermined position \( \theta_2 \). Of particular note is the fact that the frequency dependence of the anisotropy of the dielectric constant is clearly taken into account in the resulting formula (10).

In the case of a sinusoidal waveform \( V(t) = V_0 \sin(f \cdot t) \) \( (a_0 = 0, a_n = 0, b_1 = V_0, b_n = 0) \) solution takes the form:

\[
\ln \left( \frac{tg \theta_2}{tg \theta_1} \right) = \frac{\varepsilon_0 V_0^2}{2 \gamma_1 d_0^2} \left[ \Delta \mathcal{X} + \frac{\chi^{\circ}}{1 + (f \tau)^2} \left( t_i - \frac{\sin(2f \cdot t_i)}{2f} \right) + \frac{\chi^{\circ}}{1 + (f \tau)^2} \frac{\tau \cos(2f \cdot t_i)}{2} \right],
\]

(11)

where \( t_i \) - duration pulse \( V_0 \) - the amplitude of the electric field.

3. Conclusion

For HAN structure DF NLC an approximate analytical solution of equations describing the dynamics of the director reorientation under the influence of the periodic electrical signal of arbitrary shape. Calculation formulas to determine the size of the control signal to produce a symmetrical optical response of the structure HAN DF NLC. Comparison of experimental data with the results of numerical and analytical calculations showed that when modeling the optical response of the structure HAN DF NLC analytical solution is in good agreement with the experimental results in the case of small deformations of the LC layer.

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