Dependence of the integral characteristics of a nematic light modulator on the physical parameters of a liquid crystal

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Abstract. In the present work, the effect of physical constants of an LC material on the integral characteristics of a modulator operating in a waveguide mode in an LC structure with a twist angle of 270° and antisymmetric boundary conditions in the working cell was studied using the method of computer simulation. It is shown that, under antisymmetric boundary conditions, the small value of the total response time of the LC modulator is due to the absence of a “backflow” in the LC cell and the role of only half of the LC working gap thickness in the dynamics of switching between two states in such a device. In addition, it was found that in order to simultaneously achieve high contrast ratios and a short total response time of the device, it is necessary to choose an LC material with a high value of its dielectric anisotropy. In this case, there is an optimal set of elasticity constants for the LC material, which simultaneously realizes a high contrast ratio and a short total response time of the modulator.

1. Introduction
Currently, liquid crystals (LC) have found wide application in various systems for displaying and converting information [1]. The most well-known areas of use of LCD systems are all kinds of indicator and display systems [1 - 4], as well as modulators of optical radiation [3 - 7]. In connection with the development of virtual reality systems, a class of LC modulators called active 3D glasses is of particular interest [4, 8]. Usually, a high-speed LC modulator is based on various designs π - cells [9], in which LC structures with a zero or 180-degree twist angle are used, however, as recent works have shown, the LC shutter, in which an LC with an angle swirls 270° and with antisymmetric boundary conditions on orienting surfaces [10]. Such a design of an LC shutter has been known for a long time [11], but how the physical parameters of an LCD affect its characteristics at high control voltages has not yet been clarified. This work is aimed at filling this gap and presents the results of computer simulation of the characteristics of LC modulators of optical radiation.

2. Integral characteristics of LC information processing device and their modeling
Integral characteristics of LC devices can be divided into three groups: optical; electro-optical; dynamic. The integral optical characteristics of an LCD device are the characteristics averaged over the wavelength of the optical range of the signal being processed: the spectrum average transmission, the spectrum average contrast ratio (or contrast), the angular dependences of the spectrum average contrast ratio and the transmission spectrum average, color coordinates and achromaticity of the open or closed states of the modulator. The dynamic characteristics of the LC modulator include the response ($τ_{on}$) and relaxation ($τ_{off}$) times when the control voltage is switched from the “off” state to the “on” state and back. To select the optimal design of the LC modulator, it is sufficient to use a set of only four integral optical characteristics [12]:
• average over the spectrum transmission of the LC device in the "open" or "off" state. Usually this condition occurs when there is no voltage at the gate electrodes. Therefore, the spectrum average transmission of the LC modulator is denoted as $T_{\text{off}}$;
• color coordinates in the color triangle and achromaticity of the image. By achromaticity $H$ we mean the distance of the current color point of the device on the color triangle from the white point, for example, the source $D_{65}$ This characteristic describes the distance of a given point from a white point on a color triangle;
• average over the spectrum contrast ratio $C$. Its value is determined as follows:
\[
C = \frac{T_{\text{off}}}{T_{\text{on}}},
\]
where $T_{\text{on}}$ is the average over the spectrum transmission of the device in the "closed" or "on" state when voltage is applied to the control electrodes;
• total response time of the LC device ($\tau$) ($\tau = \tau_{\text{on}} + \tau_{\text{off}}$).

Usually, an LC device for converting information is considered promising for further operation if these four integral characteristics satisfy the following conditions:
\[
T_{\text{off}} \geq 35\%, \ C \geq 100: 1, \ H \leq 0.05, \ \tau \leq 6 \text{ ms}.
\]

Due to the large number of design and technological parameters that determine the characteristics of the LC shutter, for engineering practice, an idea of the features of these dependencies, as well as the search for the optimal design of such a device, can be obtained only by computer simulation [13]. In this regard, we used the MOUSE-LCD computer simulation system [14] to study the characteristics and search for the optimal parameters of the LC device. This software package makes it possible to simulate the characteristics of various LC devices with an accuracy within 10%, which usually does not exceed the experimental error, and the simulation error is mainly determined by the accuracy of specifying the physical and design parameters of the modulator.

3. Results and discussion

Earlier it was shown that at high values of control voltages the minimum total response time has a device based on an LC structure with a twist angle $\Phi_T = 270^\circ$ under antisymmetric boundary conditions [10]. The device contains an input polarizer, an LC cell, a phase compensator and an output polarizer located in series on one optical axis. The input polarizer with its maximum transmittance is oriented in the direction of rubbing on the input substrate, and the output polarizer - in the direction of rubbing on the output substrate. The thickness of the $d_L$ LC layer in the working cell is 3.5 μm. This thickness of the LC working layer was chosen because a decrease in $d_L$ leads to a violation of the waveguide regime of the LC structure and greatly deteriorates the optical characteristics of the LC modulator, and an increase in $d_L$ results in an increase in the response time of the device. Antisymmetric boundary conditions on the orienting cell substrates are due to the standard technology of rubbing the cell substrates, which provides the pre-tilt angle of the liquid crystal molecules on the input surface equal to $2^\circ$, and on the output surface $- (2^\circ)$. The phase compensator is a uniaxial phase plate oriented at an angle of 28° to the rubbing direction on the first substrate of the LC cell and having an optical thickness of 0.0345 μm. The described modulator device has the following values of integral characteristics: contrast ratio reaches 350: 1; achromaticity of the device in the "off" state $H < 0.05$; spectrum average transmission $T_{\text{off}} > 38\%$; total response time of the device $\tau \sim 6$ ms. These data indicate good optical characteristics of such an LC device for use as an LC shutter.

Let us discuss the dynamics of switching the LC modulator at different control voltages. The response time of the LC modulator is the sum of the on time and the off time. The turn-on time is the time required for the LC modulator to go from a state with zero control voltage to a state with a high control voltage. The turn-off time is the time required for the LC modulator to make a reverse
transition when the control voltage is switched from high to zero. In this case, the short response times of this LC modulator are achieved due to three factors: 1) high values of control voltages; 2) antisymmetric boundary conditions in the structure; 3) small thickness of the LC cell.

A typical dependence of the total response time ($\tau$) of such an LC modulator on the control voltage $U$ is a decreasing function. Analysis of this dependence showed that it can be approximated with an error of 15% by a simple function [15]:

$$\tau = c + \frac{a}{U^2 - b},$$

(1)

where the constants $a$, $b$, and $c$ depend on the physical constants of the LC and the boundary conditions in the LC cell (the twist angle of the structure, the pre-tilt angles of the LC molecules on the substrates). Both experimental and theoretical description of back flow effects in nematic and cholesteric liquid crystals is presented in [17-19].

A few words should be said about the effect of the “backflow” on the relaxation time, which significantly affects the dynamics of switching off the LC modulator under symmetric boundary conditions [13]. We carried out a computer simulation of the switching dynamics of an LC modulator with antisymmetric boundary conditions, and as a result, it was found that the relaxation time of such a device is the same with and without taking into account the “backflow”. It can be assumed that the short response time of the LC modulator with antisymmetric boundary conditions can be explained by two factors: 1) antisymmetric boundary conditions in the LC cell, in which only half of the working gap thickness plays a role [16]; 2) in the dynamics of switching between the two states in an LC modulator with antisymmetric boundary conditions, there is no influence of the “backflow”. The latter statement was confirmed by us by computer simulation of the dynamics of switching the LCD shutter with and without the “backflow”, which showed the same relaxation times for both cases.

Let us consider the influence of the physical parameters of an LC substance (anisotropy of the dielectric constant and elastic constants) on the characteristics of an LC modulator, the design and physical parameters of which are described in the previous section. The following values were chosen as operating voltages: $U_{on} = 8V$, and $U_{off} = 0V$.

Two integral characteristics of the modulator (average transmission in the off state $T_{off}$ and achromaticity in this state $H_{off}$) do not depend on the physical parameters of the LC substance, since this state is observed at zero control voltage and does not depend on all possible parameters and conditions. At the same time, the conditions of prospects for further use in data processing systems are met, which are superimposed on the optical integral characteristics ($T_{off} \geq 35\%, H \leq 0.05$).

In what follows, we will consider only the dependences of the spectrum-averaged contrast ratio $C$ and the total response time $\tau$ of the modulator on the physical constants of the LC material. In addition, the influence of the physical constants of the LC material on the voltage of the optical threshold of the electro-optical effect $U_{opt}$, on the basis of which the LC modulator operates, should be considered. The optical threshold voltage is the value of the control voltage in the LC cell at which the optical response changes when a certain electro-optical effect is observed. In the case of the effect of electric field-controlled birefringence in an LC, the voltage of the optical threshold coincides with the voltage of the threshold of the Fredericksz effect. In our case, the voltage of the optical threshold of the waveguide effect is significantly higher than the voltage of the Fredericksz threshold, since the observation of this effect requires a significant deformation of the LC layer in the working cell [13]. Therefore, the magnitude of the voltage of the optical threshold characterizes the degree of deformation of the LC layer in the working cell, which affects the total response time of the LC modulator.

In fig. 1 shows the dependences of $C$ and $\tau$ on the dielectric anisotropy of the LC material. As can be seen from this figure, the dependence $\varepsilon \Delta (\tau = \tau)$ with an error of 15% is described by linear regression. At the same time, an increase in the anisotropy of the dielectric constant of the LC leads to a decrease
in the total response time of the modulator due to the fact that the degree of deformation of the LC layer increases. The dependence \( C = C (\Delta \varepsilon) \) has the shape of a curve with a minimum. Thus, in the LCD modulator described above, in order to simultaneously achieve high contrast ratio values and a short total response time of the device, it is necessary to choose an LCD material with a high value of its dielectric anisotropy.

Let us consider the influence of the elasticity coefficients of the liquid crystal on the characteristics of the liquid crystal. Let \( \omega_1 = k_{33}/k_{11} \) and \( \omega_2 = k_{33}/k_{22} \). Analysis of the data shows that the behavior of the dependence \( U_{\text{opt1}} = U_{\text{opt}}(\omega_1) \) is opposite to the behavior of \( U_{\text{opt2}} = U_{\text{opt}}(\omega_2) \). In this case, the dependence \( U_{\text{opt1}} = U_{\text{opt}}(\omega_1) \) with an error of 10\% is a linear regression, and the dependence \( U_{\text{opt}} = U_{\text{opt}}(\omega_2) \) is a linear progression with the same error. This behavior of the dependencies \( U_{\text{opt1}} = U_{\text{opt}}(\omega_1) \) and \( U_{\text{opt}} = U_{\text{opt}}(\omega_2) \) is explained as follows. The magnitude of the voltage of the Fredericksz junction depends on these parameters as follows:

\[
U_{\text{Fred}} = (k_{11} \cdot (1 + C_a \cdot \omega_1 \cdot (1 - 2/\omega_2 C_b)))^{1/2},
\]

where \( C_a \) and \( C_b \) are constants determined by the LC material.

The ratio of the LC elasticity constants \( \omega_1 \) increased due to a decrease in \( k_{11} \), while the parameter \( \omega_2 \) remained constant. As can be seen from expression (2), with an increase in \( \omega_1 \), \( U_{\text{Fred}} \) decreases, which leads to a decrease in \( U_{\text{opt}} \). In turn, the ratio of LC elasticity constants \( \omega_2 \) increased due to a decrease in \( k_{22} \), while the parameter \( \omega_1 \) remained constant. In accordance with expression (2), this leads to an increase in \( U_{\text{Fred}} \), and, accordingly, \( U_{\text{opt}} \).

The dependences of \( C \) and \( \tau \) on the ratio of the elastic constants \( k_{33}/k_{11} \) and \( k_{33}/k_{22} \) of the LC material are shown in Fig. 2. As can be seen from this figure, the behavior of the dependences \( C = C(\omega_1) \) and \( \tau = \tau(\omega_1) \) is opposite to the behavior of the functions \( C = C(\omega_2) \) and \( \tau = \tau(\omega_2) \). In addition, from Fig. 2 it follows that the dependences of the contrast ratio of the total response time of the LC modulator on the ratio of the elasticity coefficients of the LC \( \omega_1 \) and \( \omega_2 \) indicate the presence of optimal values of these parameters at which the maximum possible value of the contrast ratio is reached and, simultaneously, the minimum value of the total response time of the device. The opposite behavior of the dependences \( C = C(\omega_1) \) and \( C = C(\omega_2) \) is explained by the fact that, in the opposite way, the values of the optical threshold voltages, which characterize the degree of distortion of the LC layer in the working cell, depend on these parameters. In this case, for a fixed value of the control voltage, the contrast ratio is the higher, the lower the voltage of the optical threshold, that is, the more the LC layer is deformed. The opposite behavior of the curves \( \tau = \tau(\omega_1) \) and \( \tau = \tau(\omega_2) \) is similarly explained. The
nonlinear nature of the dependences $\tau\left(\omega_1\right)$ and $\tau\left(\omega_2\right)$ can be understood on the basis of the complex influence on the dynamics of switching parameters $\omega_1$ and $\omega_2$, which does not allow obtaining simple expressions for these functions. All these dependences indicate the presence of an optimal set of elasticity constants of the LC material, at which a high contrast ratio and a short total response time of the modulator are simultaneously realized. For this, it is necessary to choose an LC material for which the value of the parameter $\omega_1$ is close to unity, and the value of the parameter $\omega_2$ is about 3.

It follows from the previous results that the values of the characteristics of the LC modulator $C$, $()$ and $U_{\text{opt}}$ should depend on the absolute value of the elasticity coefficients of the LC at constant values of the parameters $\omega_1$ and $\omega_2$. Let $K$ be the value of the average coefficient of elasticity of the liquid crystal $K = \left(k_{33} + k_{22} + k_{33}\right)/3$. Our calculations show that the dependence $U_{\text{opt}} = U_{\text{opt}}(K)$ is a linear progression with an error of 10%, which is easy to understand using expression (2). And the dependence $C = C(K)$ has the shape of a curve with a minimum, which indicates the presence of an optimal value of the average coefficient of elasticity of the liquid crystal.

The dependence $\tau = \tau(K)$, which is a monotonically increasing function, requires separate consideration. Indeed, it is known that the reaction and relaxation times are inversely proportional to the value of the LC elasticity coefficient [13]. However, we must remember that we are in the mode of a fixed value of the control voltage for the "on" state. In this mode, with an increase in the parameter $K$, the value of the threshold voltage also increases. This leads to the fact that the degree of deformation of the LC layer decreases, which, as is known, leads to an increase in the total reaction time of the modulator. This conclusion is confirmed by our calculations when fixing not the absolute value of the control voltage in the “on” state, but when fixing the voltage of the Fredericksz transition $U_{\text{nor}} = U_{\text{on}}/U_{\text{Fredericksz}}$ normalized to the threshold value. In this case, at the same $U_{\text{nor}}$ value, the full response times of the modulator are the same. The latter circumstance suggests that each LC material has its own modulator control mode. The magnitude of the control voltage and the method of switching between the "on" and "off" states should be selected based on the physical constants of the LCD and the design parameters of the device.

4. Conclusion
In the present work, the influence of physical constants of the LC material on the integral characteristics of the modulator was studied using the method of computer simulation. The device
operates in a waveguide mode in an LC structure with a twist angle of 270° and antisymmetric boundary conditions in the working cell. Shown, that:

1) under antisymmetric boundary conditions, the short total response time of the LC modulator is due to the absence of a “backflow” in the LC cell and the fact that only half of the working gap thickness plays a role in the dynamics of switching between two states in such an LC modulator;

2) for the simultaneous achievement of high contrast ratio values and a short total response time of the device, it is necessary to choose an LC material with a high value of its dielectric anisotropy;

3) there is an optimal set of elasticity constants of the LC material, at which a high contrast ratio and a short total response time of the modulator are simultaneously realized; for this, it is necessary to choose an LC material for which the value of the parameter \( \omega_1 \) is close to unity, and the value of the parameter \( \omega_2 \) is about 3;

4) for each LC material there is its own modulator control mode, and the control voltage value and the method of switching between the “on” and “off” states should be selected based on the physical constants of the LCD and the design parameters of the device.

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