[4] Analysis of optical characteristics of various designs of a classical "guest – host" LC modulator

G.V. Simonenko[1], S.A. Studentsov[2], V.A. Ezhov[3]
[1]N.G. Chernyshevskiy Saratov State University, Saratov, Russia
[2]Scientific and Production Enterprise "Photon" Ltd, Saratov, Russia
[3]A. M. Prokhorov General Physics Institute of RAS, Moscow, Russia

Abstract

Using computer modeling, the analysis of optical characteristics of a "guest —host" liquid crystal (LC) modulator is conducted. In the article, classical LC modulator designs realized on the basis of a planar cell with various LC twist angles with and without polaroid are considered. Besides, a polaroidfree LC modulator design with homeotropic LC orientation is analyzed. Practical recommendations concerning finding optimum LC modulator designs for various specific purposes are made.Keywords: computer simulation, optical characteristics, LC modulator, "guest — host" effect.

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Introduction

Liquid-crystal (LC) modulators (LCM) based on "guest-host" electrooptical effect are of great interest for information display and processing systems with increased optical efficiency due to operational possibilities of these LC modulators without polarizers (non-polaroid design) or with one polarizer only [1 – 6]. There are several liquid-crystal modulators currently in production based on "guest-host" electrooptical effect both in transmission and reflection designs [6]. The most widely used designs for these devices are implemented in the form of classical sandwich-type structures (based on various homeotropic and planar orientations of LC) [5, 6], and they are also manufactured in the form of LC dispersed in a polymer film (these devices are called polymer-dispersed-liquid-crystals – PDLC) [6]. In compare with any other "guest-host" devices the classical LC modulator, based on a single "guest-host" LC cell, has such advantages as simple technology, low manufacturing costs and a higher transmittance at a fairy high image contrast [5, 6]. Due to variety of the designs of "guest-host" LC modulators the optimization of their designs is relevant to expand their applications. The analysis of optical characteristics of the standard design of these LC modulators is carried out rather fully [5 – 7]. In this case a very large set of optical, electrooptical and dynamic characteristics is usually used to analyze such LC modulators [7 – 11]. However, questions of optimization of these LC modulators with different LC orientation structures and various types of LC cells, including various twist angles of LC structure, remain still open.

This paper is addressed to solve this problem by optimizing different kinds of classical "guest-host" LC modulators by using computer simulation.

1. Methods of research

1.1 Optical characteristics of LC modulators

As is known [7-11], for sufficiently complete theoretical and experimental description of electrooptical and optical characteristics of LC modulators it is necessary to calculate or measure a wide range of their parameters (characteristics) which primarily include:

– optical characteristics (transmittance, contrast, angular dependencies of contrast and transmittance, color coordinates);
– electrooptical characteristics (volt – contrast characteristic, multiplexing capability);
– dynamic characteristics (rise and decay times).

To describe adequately the characteristics of LC modulators it is convenient to use the following set of their optical characteristics [11, 12]: the mean value of the transmittance over the whole spectrum or at certain wavelengths under the condition ON (OFF) T_{on} (T_{off}); color coordinates in a color triangle and image achromatism; the mean value of the image contrast over the whole spectrum or at certain wavelengths; the indicatrix of the mean value of the contrast over the whole spectrum or at certain wavelengths. Under condition ON we mean such a state of LC shutter, where its control electrodes are under the voltage exceeding the threshold value. When the control voltage on LC cell electrodes is below the threshold, its state corresponds to condition OFF.

In this case the average transmittance $T_{\rm off}$ of the device over the whole spectrum under condition OFF ($T_{\rm on}$ under ON) depends on the LC modulator transmittance under condition OFF (ON) $T_{\rm off(on)\lambda}$ at the wavelength λ of the spectral distribution of the standard white light source D_{65} (or of any other radiation source) and on the spectral eye response [12].

In particular, the required image contrast should be provided while LC modulator has two optical states in the LC shutter mode. For positive images (black index on a light background) the ratio $T_{\rm off} > T_{\rm on}$ is true, for negative images (light index on a dark background) $T_{\rm off} < T_{\rm on}$. Over the spectrum the mean value of the contrast $C_{\rm pos}$ for positive images is calculated as

$C_{\rm pos}=T_{\rm off}/T_{\rm on}$,

and the mean value of the contrast of the contrast $C_{\rm neg}$ for negative images as

$C_{\rm neg}=T_{\rm on}/T_{\rm off}$.

Color coordinates (x, y) for LC modulator under condition ON or OFF in the color coordinate system (x, y, z) are determined by a standard procedure [12, 13].

The next important optical characteristic for black-and-white LC modulator is the image achromatism. The image achromatism is usually determined as the distance H between a current image point with color coordinates (x, y) and the white point D_{65} with the coordinates (x_{65}, y_{65}) [12]:

$$H=\sqrt{(x-x_{65})^2+(y-y_{65})^2}\ .$$

The indicatrix of the contrast is determined as the dependence of the image contrast on the angle φ of light incidence and on the azimuth ζ of the light incidence plane. Furthermore, the azimuth angle ζ of the light incidence plane is usually counted clockwise the direction of LC molecule orientation relatively to a front surface of LC cell. The concept of the viewing angle Ψ is often used to characterize the angle dependence of the LC modulator contrast. In our situation the viewing angle for LC modulator is the angle between two azimuth directions of the light incidence plane at the fixed angle φ of light incidence, for which the image contrast C is not less than a certain level [12].

Due to complexity of natural modeling, we used the computer simulation software system *MOUSE–LCD* [8, 11] to analyze the characteristics and find the optimal parameters of LC modulators.

1.2 Computer simulation software

The software package *MOUSE–LCD* [8] is intended for simulating electrooptical, optical and ergonomic characteristics of the following electrooptical effects and for LC structures based thereon:

– the birefringence effect in LC *supertwist nematic (STN)* structures;

– the birefringence effect in double *supertwist nematic (DSTN)* LC structures in two successive STN structures placed between two crossed polarizers;

– the birefringence effect in triple STN structures (in three successive STN cells);

– the birefringence effect in the supertwist LC structure, behind of which it is placed a phase system consisting of one or more anisotropic polymer films, whose optical axes are directed at an angle to each other and which are placed between two crossed polarizers (*neutral twisted nematic – NTN structure*);

– the twist effect (*twist nematic – TN* structure);

– the “guest-host” effect (“*guest-host*” – *GH* structure) in the various LC orientation structures;

– the “corkscrew” effect;

– the birefringence effect in π-cells.

In this case the software package allows us to calculate the following characteristics of LC modulators:

– color coordinates, transmittance spectra, the mean value of transmittance and spatial characteristics, all characteristics depending on the control voltage, elastic and dielectric constants of LC material, on the LC twist and pretilt angles, on design features of LC modulators (*TN, STN, DSTN, NTN* and *GH* structures);

– rise and decay times t_{rise} and t_{decay} of optical response of LC modulator structures depending on physical and constructive parameters of the modulators and of LC material;

– the threshold voltage of appearance of strip dielectric instability domains in LC twisted structures;

– optical characteristics of LC modulator in case of two-dimensional deformation of LC layer in electrical field at various configurations of control electrodes.
The initial software version ("ELECTROOPTICS – M") was developed at the end of the 80s for general-purpose computers series EC [14]. Somewhat later the PC software package for the version 3.0 MS DOS operating system has been implemented [15]. Design software modules included in the software packages have been written in a free available *Fortran* 77 (95) programming language, and their recompilation in the *Linux* family operating system allows one to use these software packages in the said operating system. Moreover, some certain software modules can be used independently from other to solve independent subtasks (for example, to calculate LC two-dimensional elastic deformation or LC deformation dynamics in electrical fields). Thus the modular approach has been used in the implementation of these software packages, according to which the solving an independent task requires using an independent software module designed as a separate executable module or a separate object module. In this case the connection between individual software modules can be performed only through data files. This approach to simulation of electrooptical and optical characteristics allows to consider the arbitrary designs of LC modulators wherein the effects of polarized beam interference or the "guest-host" or both of them are used. The device itself can consist either of one classical LC cell or of a combination thereof.
The software package performs a step-by-step simulation of LC modulator characteristics in the following sequence:
– calculating the LC director static field configuration in electrical fields. Problem-solving methods are described in papers [11, 16, 17];
– calculating the LC modulator static optical response under the static control voltage. Problem-solving methods are described in papers [11, 18, 19];
– calculating the LC director reorientation dynamics under the switching control voltage. Problem-solving methods are described in papers [11, 20];
– calculating the rise and decay times of LC modulator under switching control voltage. Problem-solving methods are described in papers [11, 18, 19];
– calculating the threshold voltage for strip dielectric instability domains appearance in the LC layer structure. Problem-solving methods are described in paper [21].

In computer simulation the 'sandwich'-type LC cell model is the main model. Such structure usually consists of two glass substrates with conductive and alignment layers, sequentially deposited on inner sides of substrates, and the gap between them is filled with LC material. All surfaces are parallel to each other. If the LC modulator with a polaroid is used, then the polarizer is placed outside on one of the glass plates (for example, "guest-host" LC modulator with one polarizer). In two-polaroid design of LC modulator the LC cell is placed between two polarizers (e.g. twist effect LC modulator).
Let us say a few words about mathematical methods on which the software package is based on. At the first stage of modeling, to calculate LC static deformations in electric fields we used differential equations of the LC elasticity theory [7], the solution of which is described in detail in papers [11, 16, 17]. At the second stage of modeling the LC devices, their optical characteristics are calculated by means of different methods of matrix optics described in detail in papers [11, 18, 19]. To simulate the LC switching dynamics from one state to another we used differential equations of 'Ericksen-Leslie' theory [7], the problem-solving methods for which are presented in papers [11, 20]. In this case, the dynamics of optical response of LC device is also calculated by means of matrix optics methods [11, 18, 19].
Comparison of experimental results and calculation data for twist– and "guest-host" LC modulators shows that a difference error Σ in experimental and calculation optical characteristics for given types of LC modulators are within the range of the experimental error. If the angle of light incidence onto the device varies from 0^0 to 45^0, then $\Sigma \leq 10\%$ for twist LC modulators and $\Sigma \leq 6\%$ for "guest-host" LC modulators. Therefore, the developed software provides a quantitatively correct description of electrooptical and optical characteristics of both twist– and "guest-host" LC modulators.

1.3 Design features and materials

We considered the following main structures of "guest-host" LC modulators:
– the planar LC structure with different LC twist angles (Φ_T) with polaroid;
– the planar LC structure with different LC twist angles without polaroid;
– the homeotropic LC structure without polaroid.
The planar LC structure is a structure with any twist angle of LC molecules but with pretilt angle θ_0 on

the orienting substrate that is over the range from 1^0 to 30^0. The homeotropic structure is a structure in which the tilt angle of LC molecules on the orienting substrate is over the range from 85^0 to 90^0. Let us note that the LC materials with positive dielectric anisotropy ($\Delta\varepsilon > 0$) are used in planar structures, whereas the LC materials with negative dielectric anisotropy ($\Delta\varepsilon < 0$) are used in homeotropic structures.

A large number of constructive-technological and physical parameters of LC modulators defines their optical characteristics [9, 11]. In this paper the following design parameters of LC modulators are considered: thickness d of LC layer; twist angle Φ_T of the planar structure; ratio d/p_0 of the thickness d of LC layer to the pitch p_0 of the homeotropic structure cholesteric helix; the pretilt angle θ_0 of LC molecules relative to orienting substrates for the planar LC structure. The following physical parameters of LC modulators are used: the value of anisotropy Δn of LC refraction indices; the concentration c of a dye dissolved in LC; the value of LC dielectric anisotropy $\Delta\varepsilon$.

In the simulation of electrooptical characteristics of LC modulators with the planar structure the following physical parameters for the LC material *ZLI* 4756/2 type (manufactured by Merck, Germany) are used: K_{11} = 10.5 10^{-6} dyne, K_{22} = 6.9 10^{-6} dyne, K_{33} = 16.8 10^{-6} dyne, $\varepsilon_\perp$ = 4.8, $\varepsilon_\parallel$ = 16.54, Δn (436 nm) = 0.104, Δn (546 nm) = 0.1; Δn (633 nm) = 0.096) [22]. In case of LC homeotropic orientation in the modulator the following physical parameters for the LC material *ZLI* 3200 type (manufactured by Merck, Germany) are used: K_{11} = 9.5 10^{-6} dyne, K_{22} = 6.9 10^{-6} dyne, K_{33} = 10.8 10^{-6} dyne, $\varepsilon_\perp$ = 11.3, $\varepsilon_\parallel$ = 6.54, Δn (436 nm) = 0.046, Δn (546 nm) = 0.044 Δn (633 nm) = 0.042) [22]. These physical parameters were the constants in all calculations, and the *NPF – F* 1205 *DU* film was used as the polarizer. The mixture MIB 9 (manufactured by Merck, Germany) [23] is used as a dye with the following optical parameters: dye concentration c = 1%, working thickness of LC layer d = 9 μm, dichroic ratio D = 11,7.

Also the following constructive parameters of LC modulator are used: the 1st passivation layer with thickness of 0.11 μm and with the refraction index of 1.45 value; the electrode layer with thickness of 0.06 μm and with the refraction index of 2.0 value; the 2nd passivation layer with thickness of 0.11 μm and with the refraction index of 1.45 value; the orienting layer with thickness of 0.02 μm and with the refraction index of 1.4 value.

It is known [9] that electrooptical characteristics of "guest-host" LC modulators are largely determined by changing the optical density of working material from the maximum value $D_\parallel$ to the minimum value $D_\perp$. In this case the optical densities depend on constructive and physical parameters of LC modulator as follows:

$D_{//} = \alpha_{//} cd$, $D_\perp = \alpha_\perp cd$,

where $\alpha_{//}$ and $\alpha_\perp$ are respectively the maximum and minimum extinction coefficients of working material; c is the dye concentration that usually does not exceeds 3 %; d is the thickness of LC layer.

Besides, the dependence of the maximum dye absorption on the control voltage strongly influences on characteristics of "guest-host" LC modulator. Therefore, the following analyzed characteristics are chosen under ON-condition: the mean values of the image contrast C and the transmittance T_{on} over the spectrum depending on physical parameters of LC modulator (dye concentration c, anisotropy Δn of refraction indices of LC layer, dielectric anisotropy $\Delta\varepsilon$ of LC layer) and on its design parameters (thickness d of LC layer, twist angle Φ_T of LC structure for LC planar orientation, ratio d/p_0 of the thickness d of LC layer to the pitch p_0 of the cholesteric dopant for LC homeotropic orientation, the pretilt angle θ_0 of LC molecules on orienting substrates for LC planar orientation). Moreover, optical response times for LC modulators were also analyzed depending on the same parameters.

Notice that one of the main optical characteristics of LC modulators is the contrast ratio indicatrix [7, 9-11]. However, as is said earlier [9], angle dependences of the image contrast of "guest-host" LC modulators are poorly expressed, and the shape of the contrast indicatrix is close to the shape of a circle. At the same time the image contrast values for incidence angles within the range of 10^0 – 70^0 differ not more than by 20% from the contrast values for the normal incidence (for the maximum contrast value) [9]. Therefore, this paper does not involve any data on angle dependencies of the image contrast on various parameters of LC modulator.

The next sections of this paper give the results of computer simulation of "guest-host" LC modulators for the following three types of LC structures:

– LC planar structure with one polaroid at various twist angles;

– LC planar structure without polaroid at various twist angles;

– LC homeotropic structure without polaroids.

Notice that the first two designs provide the negative image whereas the third design – the positive image.

2. Results and discussion

2.1 LC modulator based on planar structure with one polarizer

Fig. 1 shows the LC modulator image contrast dependence on anisotropy Δn of the LC refraction index for various thicknesses d of LC layers with the 90^0 twist angle of LC molecules. It is seen that liquid crystals with large Δn values should be used in such LC modulators, because low Δn values cause violation of the Mogen waveguide mode [7, 9] and consequently decrease light absorption under condition OFF. At the same time there is no such dependence under condition ON as LC is isotropic under this condition. Therefore, the image contrast C is increased with the increase of the LC refraction index Δn.

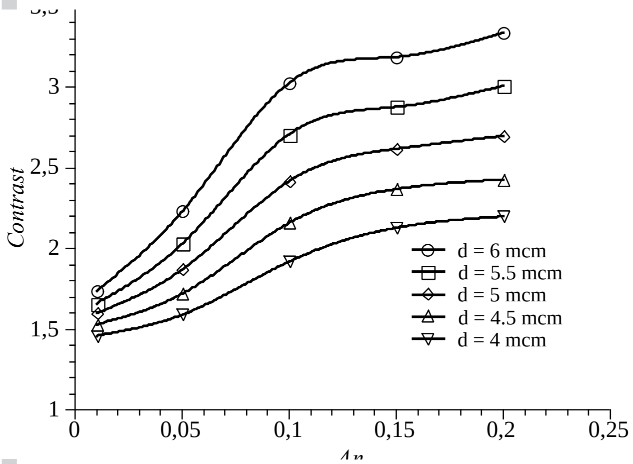

Fig. 1. Dependence of the image contrast C on anisotropy Δn of the refraction index (c =1,1 %, Φ_T = 900)

Fig. 2 shows the image contrast dependencies on the concentration c for LC modulator based on the 90^0 twist angle structure. According to expectations, LC modulator with higher dye concentration c has higher optical characteristics due to the fact that T_{on} is less dependent on the concentration c than T_{off}. The dependence $T_{off}(c)$ is strong and monotonically decreasing. At the same time the transmittance coefficient T_{off} under condition ON is changed from 38% to 29% while changing the dye concentration c from 1 to 3% and increasing the thickness d in accordance with the Bouguer law. The similar behavior of the image contrast C dependence on the LC layer thickness d. It can be easily understood, if remember that the dye optical density $D_{//,\perp}$ depends on the product cd. In this case the value T_{on} is weakly dependent on the thickness whereas the dependence $T_{off}(d)$ is strong and monotonically decreasing.

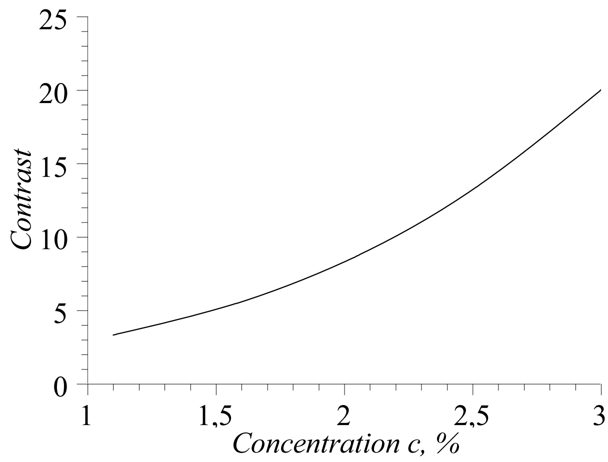

Fig. 2. Dependence of the image contrast C on the dye concentration c (d = 6 μm, Dn = 0.2, Φ_T = 900)

The LC modulator image contrast and transmittance dependencies on LC dielectric anisotropy are very weak under ON-condition. This is due to the fact that under condition OFF (when the control voltage is lower than the voltage threshold) the LC transmittance does not depend on $\Delta\varepsilon$ and under condition ON the control voltage significantly exceeds the threshold value, and also in this state the transmittance weakly depends on $\Delta\varepsilon$ [9].

Fig. 3 shows the dependence of the image contrast C of LC modulator on the twist angle Φ_T of LC structure. While changing Φ_T over the range from 0^0 to 90^0, this dependence is poor, and while further increasing Φ_T, the contrast is decreased because under condition OFF the Mogen waveguide mode is violated. This can cause increasing the LC modulator transmittance value T_{off} while transmittance T_{on} is practically independent of the twist angle of LC structure. Therefore, the image contrast C is decreased as the value Φ_T is increased.

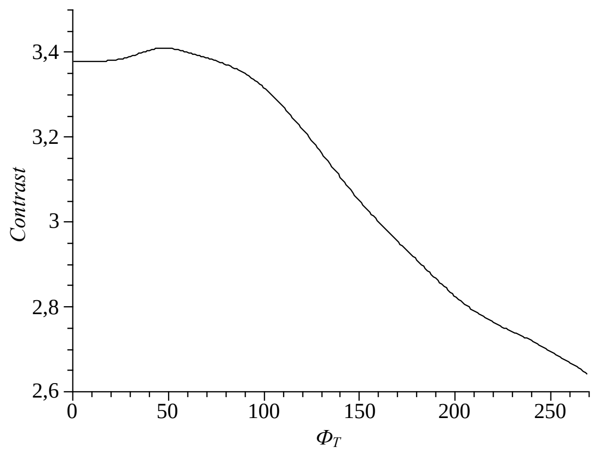

Fig. 3. Dependence of the image contrast C on the twist angle Φ_T of LC structure (d = 6 μm, Δn = 0.2, c = 1.1 %)

The similar behavior is also for the dependence of the image contrast C and transmittance T_{on} on the pretilt angle θ_0 for LC molecules on substrates of LC modulators. The value T_{on} does not almost depend on θ_0 as the control voltage significantly exceeds the threshold value in this state and is independent of the pretilt angle θ_0. The dependence $C(\theta_0)$ is slightly decreasing as the transmittance T_{off} under condition OFF is slightly increasing within the determined limits of changing the pretilt angle θ_0 [9].

2.2 LC modulator based on planar structure without polarizer

The design of "guest-host" LC modulator without polaroid has its own advantages and disadvantages. The advantages include the high transmittance level under condition ON, and the disadvantages – low image contrast. However, while using various twisted LC structures, it is possible to obtain simultaneously the transmittance level of 50 – 60% and the contrast level of 5 : 1. Fig. 4 shows the dependence of the image contrast C on the anisotropy Δn of the LC refraction index. Unlike the design with polaroid it is necessary to use in the considered design the LC material with minimum Δn value to provide the maximum image contrast, because in this case it is necessary to violate the Mogen waveguide mode to provide the maximum light absorption under condition OFF.

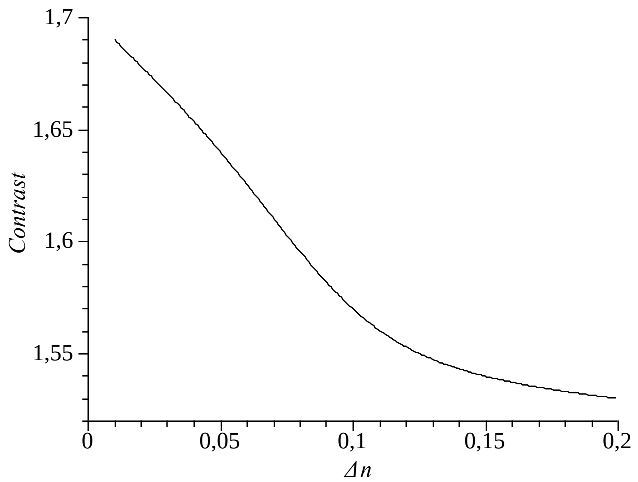

Fig. 4. Dependence of the image contrast C on anisotropy Δn of the LC transmittance index (Φ_T = 900, d = 6 μm, c = 1.1%)

The dependencies (C, T_{on}) of optical characteristics of LC modulator on the thickness d of LC layer and on the dye concentration c are the same as the similar dependencies for LC modulators with polaroid. The difference is only the image contrast level but the behavior of these curves has the same explanation.

Fig. 5 shows the dependence of the image contrast on the twist angle Φ_T of LC planar structure. As is seen, the maximum image contrast is achieved at $\Phi_T = 180^0$. It can be explained by the fact that under condition ON the transmittance of LC modulator does not almost depend on the twist angle as the control voltage significantly exceeds the threshold value. Under condition OFF the maximum light absorption corresponds to $\Phi_T = 180^0$ as this twist angle conforms with all possible linear light polarization states which can be absorbed by dye molecules oriented by their maximum absorption axes along the direction of the incident light polarization.

As for LC modulator with polaroid, the value T_{on} does not depend upon θ_0 as the control voltage in this state significantly exceeds the threshold value and does not depend on the pretilt angle θ_0. The dependence $C(\theta_0)$ is slightly decreasing as the transmittance under condition OFF is slightly increasing over the specified range of changing the pretilt angle [9].

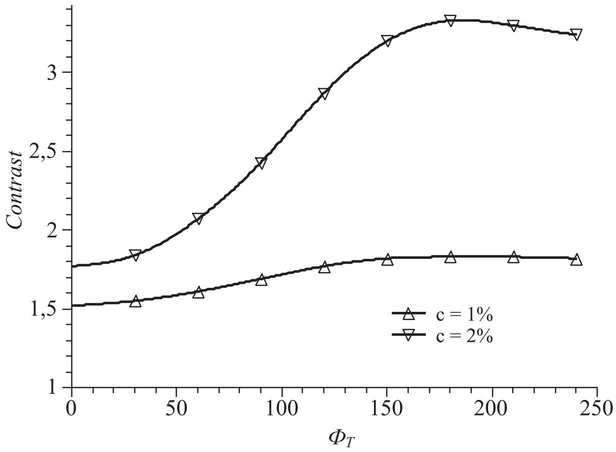

Fig. 5. Dependence of the image contrast C on the twist angle Φ_T of LC structure (Δn = 0.01, d = 6 μm)

The represented dependencies of the image contrast C and the transmittance T_{on} on dielectric anisotropy $\Delta\varepsilon$ are the same as the similar dependencies as for LC modulator with polaroid, however the contrast value C is about twice less due to higher transmittance T_{off} values.

Finally, we will analyze temporary characteristics of LC modulator based on planar structure. The dynamics of LC modulator is basically determined by physical parameters of the design and does not depend upon availability or lack of the polarizer, therefore all data given below can be referred to both designs of LC modulator. Main design parameters of LC modulator, which have considerable influence on switch-on τ_{rise} and switch-off τ_{decay} times, are the thickness d of LC layer and the ratio d/p_0 [7,9]. In accordance with the known analytical dependencies [9], τ_{rise} and τ_{decay} are increasing while increasing the thickness d

$$\tau_{rise}, \tau_{decay} \approx Gd^2,$$

where G is a constant that depends only on physical constants of LC material substance for the given value of the control voltage.

Therefore, under other conditions being equal the LC modulator with 4 micron LC layer is faster (about in 2.5 times) than the device with 6 micron LC layer.

Influence of the twist angle Φ_T on the response time of LC modulator is presented in Table 1 simply as the quality dependence, because the complete set of physical and technical parameters, which are basically unknown for most devices, is required to determine exact quantitative relationships.

Table 1. Qualitative dependency of the response time of LC modulator on the twist angle ΦT of LC structure

ft, deg.	90	180	210	225	240
$\tau=\tau_{rise}+\tau_{decay}$, msec	195	195	195	250	300

Influence of physical parameters for LC material on the response time of LC modulator is well described by the known analytical relationships [9]

$$\tau_{rise} \approx \gamma/\Delta\varepsilon, \ \tau_{decay} \approx \gamma/k,$$

where γ is the viscosity index, k is the average elasticity coefficient of LC material. Therefore, it is necessary to use LC material with low viscosity and with large value of dielectric anisotropy and elasticity coefficients to obtain small optical response times.

2.3 LC modulator based on homeotropic structure without polarizer

As shown by researches, all functional relationships of optical characteristics of "guest-host" LC modulator based on homeotropic structure without polarizer are the same as similar relationships of LC modulator based on planar structure without polarizer, and they have the same explanation. However, it should be taken into account that in case of homeotropic structures the role of the twist angle Φ_T for the structure is played by the relationship d/p_0, and the equilibrium twist angle Φ_T for LC structure is determined as

$$\Phi_T = \frac{d}{\pi p_0} 180$$

All functional relationships of optical characteristics, and physical and technical parameters of LC modulators based on homeotropic structure are given in Fig. 6, 7 and 8.

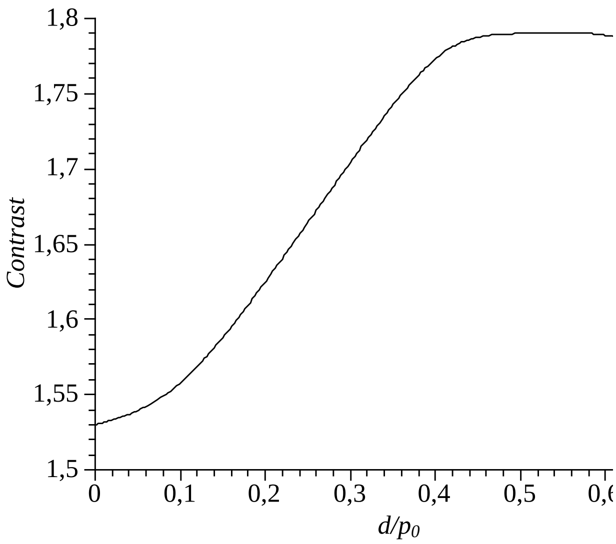

Fig. 6. Dependence of the image contrast C on the ratio d/p_0 (Δn = 0.01, d = 6 μm, c = 1.1%)

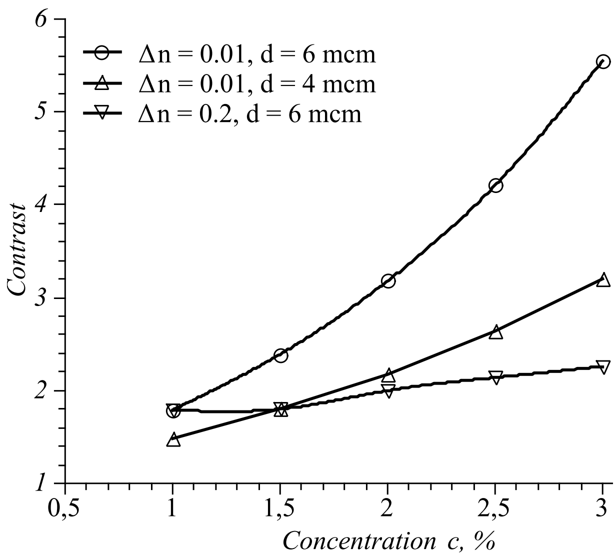

Fig. 7. Dependence of the image contrast C on the dye concentration c (Δn = 0.01, d = 6 μm, d/p_0 = 0.5)

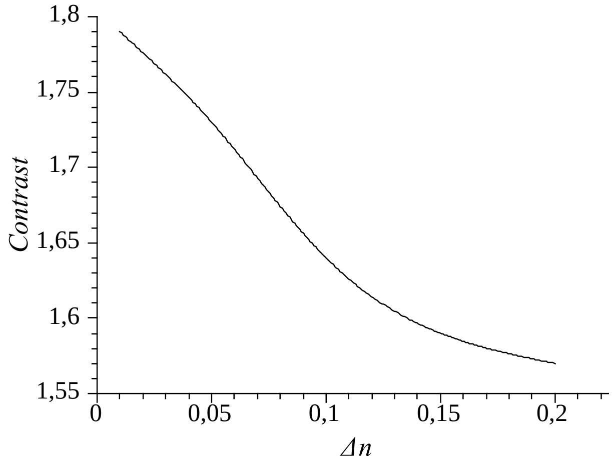

Fig. 8. Dependence of the image contrast C on anisotropy Δn of the refraction index (c =1.1 %, d/p_0 = 0.5, d = 4 μm)

Conclusion

We can draw the following conclusions on the results of carried out computer simulation of optical characteristics of "guest-host" LC modulators.

1. At small dye concentrations ($c \sim 1\%$) the optical characteristics of LC modulators with one polarizer have some minor advantages in compare with non-polaroid LC modulators.

2. LC modulators with one polarizer have significantly higher image contrast in compare with non-polaroid LC modulators while increasing the dye concentration up to the maximum possible values ($c \leq 3\%$). Also in all indicated cases the LC structure with 180^0 twist angle should be used to improve the image contrast.

3. It is necessary to use LC with larger Δn for LC modulators with polarizer and with ultralow Δn for non-polaroid LC modulators.

4. According to optical characteristics, the non-polaroid LC modulator based on planar structure does not differ from LC modulator based on homeotropic structure, only the first structure gives the negative image, and the second – the positive one.

5. According to optical characteristics, LC modulator with thin LC layers ($d \sim 4$ μm) is about 1.5 times worse in compare with one with thicker layers ($d \sim 6$ μm). In this case the response of the first one is approximately twice faster in compare with the second one. Therefore, at maximum possible dye concentrations it is preferably to use LC modulators with thinner LC layers to have the fastest response.

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