The thermo-electro-optical effect: influence of the external and material parameters on the colours' succession

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In this paper we perform a systematic study of the influence of the external and material parameters on the colour's succession, purity and intensity for the thermo-electro-optical effect. This study is based on a theoretical model for the observed phenomenon in a computer simulation of the effect. In order to simulate the thermo-electro-optical effect we have designed a computer programme, in BORLAND DELPHY 6.0 language. Our programme (THEO) validates the theoretical model and may be used to find the optimal set of parameters in order to obtain a desired succession of colours, with higher purity and intensity, for a given mixture. The results of our study could be used to enhance the performances of the optoelectronic devices based on this effect.

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1. Introduction

The thermo-electro-optical effect was discovered by M. Socaciu and co-workers and was already used in an optoelectronic device [1]. This effect appears in a mixture of the smectic liquid crystal terephtal-bis-butyl-aniline (25% TBBA) and the cholesteric liquid crystal cholesteryl myristate (75% CM) and consists in a succession of transmitted colours through the LC cell, when it is subjected to a d.c. electric field and a sine-shape variation of the temperature around a particular value [2].

Until now, we have proposed three theoretical models in order to explain the experimentally observed phenomena [3-5]. The theoretical model which fits best the experimental data is based on the theory of multiple layer interference of the ordinary and extraordinary rays passing through the layered structure of the smectic chiral mixture. The appearance of the colours was explained using the three-chromatic synthesis method [6].

The liquid crystal display performances depend on the colour parameters (intensity, purity, contrast, etc.), thus, it is extremely useful to find the optimal experimental conditions for maximum performances. Certain experimental conditions are difficult to be changed or imply a long time preparation. To avoid these difficulties we have designed the computer program THEO, which was used to validate the theoretical model, too. When a material parameter is variable, THEO simulates the behaviour of another possible liquid crystal mixture which exhibits another succession of colours.

2. Experimental

The LC cells were prepared using the conventional techniques for electrical investigations [7]. The LC textures, under different electric field and temperature values, were observed and recorded using the experimental set-up and techniques in detail reported in [8]. If the sine-shape variation of the cell temperature has the form

$$\Gamma(t) = T_0 + \Delta T \sin \omega_T t$$
, $T_0 = 67^{\circ}C$, $\Delta T = 1^{\circ}C$, $\omega_T = 4.6 \times 10^{-2} \text{ rad/s}$

and a d.c. electric field was simultaneously applied on the sample, the colours' succession rigorously follows the temperature variations. So, when the temperature has a maximum the transmitted colour is blue, while in the temperature minimum the observed colour is always red, passing through green and yellow (at intermediary temperatures).

3. Theoretical model

The observed phenomenon was ascribed to the polychromatic interference between the ordinary and extraordinary rays emerging from the anisotropic system, illuminated with white light.

The first hypothesis for theoretical modelling refers to the spatial configuration of the LC molecular director inside the LC cell. We supposed that the director undergoes a complex spatial rotation as a result of the electric field action and of surface interactions. The position of the LC long molecular axis may be described, in every point of the LC cell, by the azimuthal and tilt angles as shown in Fig. 1.



Fig. 1. a) LC cell geometry and the molecular director rotation as a result of electric field and surface interactions; b) Molecular director direction in the layers "i-1" and "i" and the angles used in the theoretical model.

We assumed, for simplicity, that the tilt angle has a symmetrical distribution inside the LC cell, along the normal to the glass plates, with a maximum value at the middle plane of the cell.

The second hypothesis is that the LC has layered structure, inside each layer the molecular director having the same orientation. Passing from one layer to another, the molecular director orientation varies. Each layer is considered to be biaxial.

As previously mentioned [5] for the explanation of the TBBA:CM mixture behaviour we have assumed that the thermo-electro-optical effect appears near a phase transition temperature. In addition, we assume now that the phase transition is of the second order.

Finally, we consider that the sine-shape variation of the temperature induces a sine-shape variation of the mixture birefringence

$$\Delta n = \Delta n_0 + \delta n \sin\left(\omega_T t + \phi_n\right).$$

With these considerations, we have found for the transfer matrix the following expression [8]

$$\left[1 - \left(\frac{l\pi\Delta n}{\lambda}\right)^2 \cdot \frac{N}{2} \cdot \left(1 + \frac{\sin 2\gamma_{N/2}}{2\gamma_{N/2}}\right)\right] \cdot \left(\frac{\cos(\sum \alpha_i)}{-\sin(\sum \alpha_i)} \frac{\cos \Delta \phi_i \sin(\sum \alpha_i)}{\cos \Delta \phi_i \cos(\sum \alpha_i)}\right).$$

where l is the molecular length, Δn is the LC birefringence, λ is the light wavelength, N is the total number of LC layers inside the cell, and $\Delta \phi$ is the phase difference between the ordinary and extraordinary rays emerging from one layer.

For further calculations we use the following experimental data: $\Delta n_0 = 0.12$; $\delta n = 0.019$; $\omega_T = 4.6 \times 10^{-2}$ rad/s; $\omega = \pi/2$;

$$1=2\times10^{-9}$$
m; $t \in (0 \div 136.5)s$.

We have used the three chromatic synthesis method in order to obtain the colours' succession based on the theoretical model [5]. It was found that the "theoretical" colours' succession is identical with the experimental observed one [7].

4. Computer simulation

The computational programme, named THEO (**TH**ermo-**E**lectro-**O**ptical), was design in BORLAND DELPHY 6 language and enables us to simulate the effect for different imaginary experimental conditions [9]. It displays: the succession of the colours in time, as a curve on the colour diagram ("trace" mode); the 3D representation of the light intensity emerging from the system, as function of wavelength and time ("grid" mode, Fig. 2).



Fig. 2. THEO working in the "grid" mode.

The computational simulation shows that the external parameters have the following influence on the colours characteristics:

- the electric field variation does not change the succession of the colours. This parameter strongly influences the transmitted light intensity, which increases for increasing electric field. A saturation phenomenon was also noticed.

- the cell thickness also influences the transmitted light intensity as shown in Fig. 3. The transmitted colours have higher purity for thicker cells. The succession of the colours is relatively weakly influenced by this parameter. Significant changes may be observed only for cell thicknesses unusual in real experimental conditions.

The material parameter contributions are:

- the molecular length has a strong influence on the succession of the colours. When this parameter decreases, the small wavelength colour is inhibited, onto a single transmitted colour (red with low purity) appearance, unaffected by the time variation of the temperature. A weak influence on the colour intensities was also observed.

- when the birefringence at zero electric field, Δn_0 , is smaller than 0.11 the blue colour in the maximum temperature disappears being replaced by the cyan colour. For Δn_0 higher than 0.13 red colour in the minimum temperature is replaced by orange. The colour intensity is weakly affected by this parameter variation.

- for small values of the pretilt angle, γ_0 , the mixture displays the entire succession from blue to red. At higher γ_0 the high wavelength colours disappear, starting with blue.



Fig. 3. Transmitted light intensity for two cells with different thicknesses (N -the number of LC layers).

These simulations are very important to set the optimum experimental conditions in order to obtain the desired result. The computational programme may be also used to anticipate the behaviour of other LC mixtures

5. Conclusions

The influence of the external and material parameters on the succession, intensity and purity of the colours transmitted by a LC cell in the thermo-electro-optical effect, was performed using a computational simulation. This simulation is based on a theoretical model and on the three-chromatic synthesis method. The external d.c. electric field has the main influence on the colour intensities, whereas the succession of the colours is strongly influenced by the material parameters.

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