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Channeled spectra simulation of an anisotropic poly-(phenylmethacrylic) ester of cetyloxybenzoic acid in tetrachloromethane

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The values of the birefringence Δn in the visible range of a 10^7 molecular weight poly-(phenyl methacrylic) ester of cetyloxybenzoic acid (PPMAECOBA) in tetrachloromethane (TCM) liquid crystal was determined from the channelled spectra of thin layers, as previously described. The spectral composition of the emerging light from a device consisting by a thin liquid crystalline layer placed between the crossed polarizers is investigated using 3-D representations in Matlab. The proposed method permits to establish the spectral composition for a given thickness of the anisotropic layer. The thickness of liquid crystalline layer for which the channels or the maxima of a monochromatic radiation are obtained could also be estimated.

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1. Introduction

The modern devices based on colour display uses liquid crystalline layers kept between two transparent protective plates [1-4] covered (on their internal faces) with transparent conducting films that facilitates the applying of an external electrostatic field between them [5].

The modern display is based on the two possible geometries of the uniaxial liquid crystalline layers: a homeotropic one, with mesogenic molecules having their long axes perpendicular on the protective plates, and a homotropic one, with mesogenic molecules oriented parallel to the plate surface. The two geometries can be realized by using some anchoring procedures [4] of the mesogenic molecules.

The mesogenic molecules are oriented parallel to the field intensity, when the liquid crystal is characterized by a positive electric susceptibility, $\Delta\varepsilon > 0$, while when $\Delta\varepsilon < 0$ they are oriented perpendicularly on the plate surface. Thus, the external electric field can improve the degree of order in the anisotropic layer, or it can disorganise the allignement of the mesogenic molecules [5].

When the initial orientation of the mesogenic molecules is perpendicular on the plates, the liquid crystals having $\Delta\varepsilon > 0$ improves its orientation along the nematic director. On the other hand, when the initial orientation of the mesogenic molecules is parallel to the plates, the external electrostatic field changes the molecular orientation of the substance, rotating its mesogenic molecules with 90 degrees.

When the liquid crystalline layers are used between two crossed polarizers, two situations could be obtained if the device is illuminated by a monochromatic radiation [6,7]:

- total extinction is obtained when the mesogenic molecules are oriented perpendicularly on the plates;
- monochromatic light is obtained after the second polarizer, when the mesogenic molecules are parallel to the plates. The radiant intensity is maxim when the nematic director makes 45 degrees with the transmission directions of the polarizers.

The device consists of two crossed polarizers and the liquid crystalline layer between them having its director at 45 degrees compared with the transmission direction of the polarizers. When this device is illuminated with visible radiation, the emerging from the liquid crystalline layer visible components have a changed polarization state, thus the spectral composition of the emergent light from the device differs from that of the incident light [8-10].

The spectral changes in the light composition depend both on the thickness and on the birefringence of the liquid crystalline layer. For a given liquid crystal we can estimate, by using a program written in Matlab, the thickness of the anisotropic layer corresponding to a given spectral composition of the emergent light.

2. Theoretical

An anisotropic uniaxial substance is characterised by two values of the refractive index when it is related to the main axes of coordinates [6,7]. The ordinary value (n_o) is measured for radiation having the electric field intensity perpendicular to the optical axis, while de extraordinary value (n_e) is measured for radiation having its electric field intensity parallel to the optical axis [10,12].

The birefringence [6,13] is defined as being the difference:

$$\Delta n = n_e - n_o \qquad (1)$$

When light propagates along a main direction of the anisotropic layer (different from the optical axis), a path difference expressed by relation (2) is introduced between the two linearly components of light acting parallel to the other two main directions.

$$(\Delta) = (n_e - n_o)L = \Delta n \cdot L \qquad (2)$$

Let us suppose that light propagates along *ob* axis (Fig. 1) of the main system of coordinates (*oabc*), the thickness of the layer measured along the propagation direction being L.

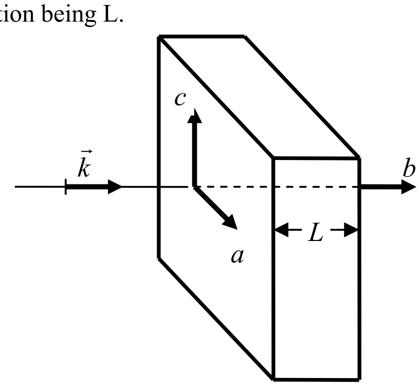

Fig. 1. Main polarization directions of the anisotropic laye.

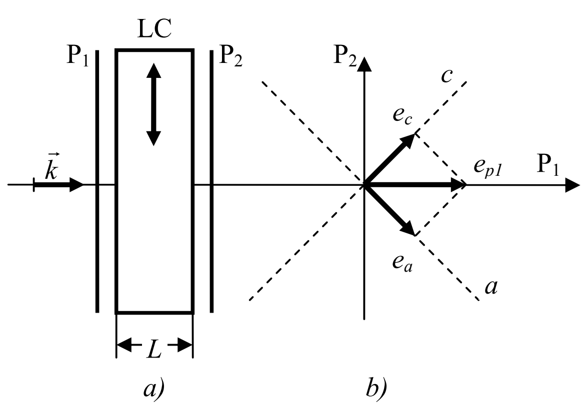

Fig. 2. a) Schematic representation of the optical device that change the polarization state; b) Relative orientation of the main axes of the liquid crystal (LC) and the transmission directions of the polarizers P_1 and P_2.

Usually the liquid crystalline layers are placed between two crossed polarizers [8-13], such in Fig. 2*a*. Thus, at the entrance of the anisotropic layer, radiation is linearly polarized having its electric field intensity parallel to the transmission direction of P_1 (Fig. 2*b*). The components $\vec{e}_a$ and $\vec{e}_c$ of the electric field intensity acting parallel to the main axes of the liquid crystalline layer are parallel to the basic directions of polarization and they do not change their polarization state in the propagation process. The corresponding main refractive indices of the layer for these components are: $n_a = n_o$ and $n_c = n_e$. At the emergence face of the layer, the two components interfere; giving radiations whose polarization state is dependent on the phase difference of the components.

$$\Delta\Psi = 2\pi\overline{\nu}_0 (n_e - n_o)L \qquad (3)$$

The phase difference $\Delta\Psi$ depends on the wavenumber of radiation directly by $\overline{\nu}_0$ and indirectly by the dispersion of birefringence.

At the emergent surface of the anisotropic layer, the components e_a and e_c are written by using the Maxwell's equation solutions:

$$\begin{aligned} e_a &= E_a \cos\left(\omega \cdot t - \frac{2\pi}{\lambda_0} n_a L + \Psi_{0a}\right) \\ e_c &= E_c \cos\left(\omega \cdot t - \frac{2\pi}{\lambda_0} n_c L + \Psi_{0c}\right) \end{aligned} \qquad (4)$$

Let be:

$\Psi_a(t, L, \nu_0) = \omega \cdot t - \dfrac{2\pi}{\lambda_0} n_a L + \Psi_{0a}$, and

$\Delta\Psi_{a,c} = \dfrac{2\pi}{\lambda_0}(n_e - n_o)L + \Delta\Psi_{0a,c}$ (phase difference at distance L in the anisotropic layer;

$$\Delta\Psi_{0a,c} = \Psi_{0c} - \Psi_{0a} \qquad (5)$$

(phase difference at the entrance of the layer)

Relations (4) can be re-written as relations (4'):

$$\begin{aligned} e_a &= E_a \cos[\Psi_a(t, L, \nu_0)] \\ e_c &= E_c \cos[\Psi_a(t, L, \nu_0) + \Delta\Psi_{a,c}] \end{aligned} \qquad (4')$$

After polarizer P_1, light is linearly polarized and one can consider

$$\Delta\Psi_{0a,c} = 0 \qquad (6)$$

The equation of the polarization ellipse is obtained from relations (4') by eliminating the momentan phase $\Psi_a(t, L, \nu_0)$ of the component e_a.

$$\left(\frac{e_a}{E_a}\right)^2+\left(\frac{e_c}{E_c}\right)^2+2\frac{e_a e_c}{E_a E_c}\cos\Delta\Psi_{a,c}=\sin^2\Delta\Psi_{a,c} \quad (7)$$

>From (7) it results the following situations [10,13]:

a) If $\Delta\Psi_{a,c}=2m\pi, m=0,1,2,...$ the linear polarized waves do not change their azimuth and do not pass through the device.

b) If $\Delta\Psi_{a,c}=(2m+1)\pi, m=0,1,2,...$ radiations change their azimuths and emerge from the device at maximum intensity, if the initial azimuth equalises 45 degrees.

c) If $\Delta\Psi_{a,c}=(2m+1)\frac{\pi}{2}, m=0,1,2,...$ radiations become circularly polarized and emerge through the device at half of the maximum intensity.

It results that, depending on the birefringence values, the thickness of the anisotropic layer could be estimated, so that the emergent light from the device has a desired spectral composition. If the anisotropic layer is thick enough, a channelled spectrum, characterized by maxima and minima is obtained in the visible range. The channelled spectra can be simulated by computer in 3D-representation of the transmission factor of the device drawn in Fig. 2.

The channelled spectra [10,13] are obtained by simulating the transmission factor of the device as function of wavenumber and birefringence or as function of the anisotropic layer thickness and birefringence.

$$T=\frac{1}{2}(1-\cos\Delta\Psi) \quad (8)$$

Relation 3 for $\Delta\Psi_{a,c}$ shows as in the channelled spectra simulation the birefringence dispersion must be taken into consideration. 3D-representations for the liquid crystals, with known values of the birefringence in the visible range (determined by experimental means) have been realized.

The obtained graphs can be used in order to vary the nuance and the brightness of the color if the birefringence is modified by applying an external electric field on the protective plates containing the liquid crystalline layer.

3. Results

The relation (8) was used to calculate in Matlab the transmission factor matrix $T(\bar{\nu},\Delta n)$ - for a given thickness of the liquid crystal layer L, and $T(\Delta n, L)$ - for a given wavenumber, respectively. Consequently, a 3D-representation was plotted for each of the two matrices obtained as mentioned above using the *mesh* function in Matlab.

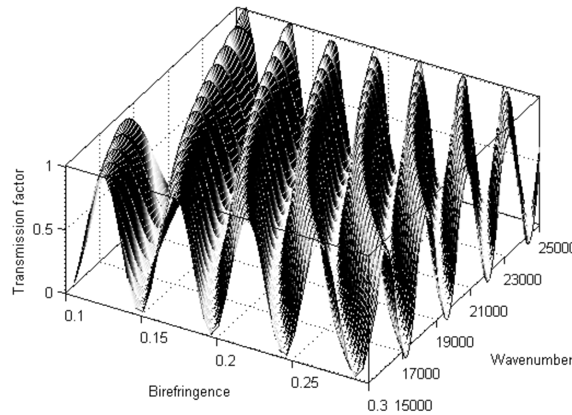

Fig. 3. Transmission factor (T) vs. birefringence (Δn) and wavenumber (ν_0) at a given thickness of the liquid crystal layer (L=14 μm).

The lyotropic liquid crystal PPMAECOBA in TCM ($10^{-2}g/cm^3$), for which we have enough information about the visible birefringence [10,11] was used in this study.

The 3D-graph obtained for $\Delta n\in[0.1, 0.3]$, $\nu_0\in[15000, 25000]\,cm^{-1}$ and L=14 μm is given in Fig. 3. The values of the wavenumber and of the birefringence for which channels are obtained can be established from Fig. 3.

For the yellow radiation of a Na lamp

$$(\nu_0=16969.28\,cm^{-1}), \Delta n\in[0.1, 0.3]$$

and $L\in[14, 20]\mu m$ the obtained 3D-graphs for the transmission factor of the device is illustrated in Fig. 4. From this graph one can establish the thickness of the layer for which a given material (with a given Δn) determines a desired number of channels of the monochromatic radiation.

From these representations we can find, for each liquid crystalline layer (having a known birefringence dispersion), the wavenumbers of the monochromatic radiations corresponding to the channels, to the maxima of radiant intensity, or to the desired intermediate values of the intensity. In accordance with theoretical notions mentioned above, the polarization state of the monochromatic radiations corresponding to minima and maxima of intensity can be established.

The simulation program permits to change the limits of the birefringence and/or the layer thickness in order to obtain a smaller number of channels in the visible range. Consequently, the spectral composition of the emergent light from the above described device can be changed.

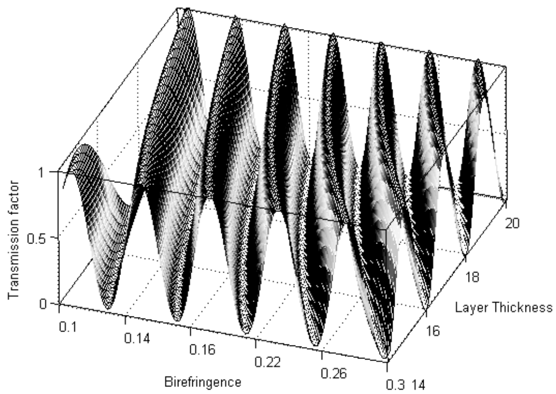

Fig. 4. Transmission factor (T) vs. birefringence (Δn) and thickness of the liquid crystal layer (L) (ν_0) at a given wavenumber ($\nu_0 = 16969.28\ cm^{-1}$).

This kind of representation is also important when we must select the nature of the uniax liquid crystal in the device described in Fig. 2 in order to obtain a desired spectral composition of the emergent light.

External fields can be estimated in order to obtain a given birefringence for a given liquid crystal that have a known dependence of the birefringence as function of the external field intensity.

4. Conclusions

This study is very important when the change in the polarization state of the visible radiations must be done in a desired way. Only some monochromatic radiations, with a desired intensity, emerge from the device consisting from two crossed polarizers and the anisotropic liquid crystalline layer between them, as Fig. 2*b* shows, for a given thickness of the layer.

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