



Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl20>

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Version of record first published: 05 Apr 2011

To cite this article: Nicolas Gallé & Mimoun Ismaïli (2008): Numerical and Experimental Dynamical Studies of Electro-Optical Response of Twisted FLC SmC* Cells, *Molecular Crystals and Liquid Crystals*, 494:1, 68-78

To link to this article: <http://dx.doi.org/10.1080/15421400802430109>

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Numerical and Experimental Dynamical Studies of Electro-Optical Response of Twisted FLC SmC* Cells

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We report electro-optical studies of twisted SmC (TSC) cell with high spontaneous polarization which is known to exhibit a V-shape like switching profile. In this study we are particularly interested in the influence of both polarization and ionic charges on the transmitted light intensity. Experimental studies show that the V-shape profile can be strongly affected because of the contribution of the ionic field to the internal one. Indeed, we show that the V-shape can be either distorted and/or sometimes shifted by the ionic field. The developed theoretical model shows that these effects are related to the azimuthal angle distribution in the cell following the ionic charges redistribution. Our studies explain firstly how the azimuthal angle distribution is modified in the presence and in the lack of ions impurities in the cell and secondly how the transmitted light intensity is affected. The reported numerical results show a good agreement with experimental one.*

Keywords: electric field; ferroelectric; ions; twist; viscosity; V-shape

1. INTRODUCTION

Among several advantages of the ferroelectrics liquid crystals devices over the conventional nematics ones, high speed of operation and bistable device configuration [1–5]. The most common electro-optical studies concern surface-stabilized ferroelectric liquid-crystals cells in planar configuration. The major problem of these devices is the lack of gray-scale capability. Several solutions were proposed to overcome this problem. Nowadays, many groups work particularly on the

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behaviours of devices with a V-shape electro-optical response [6–12]. In 1991, Patel studied another kind of planar cells where the rubbing directions of the electrodes are perpendicular to each other [13]. He used a material in the SmC* phase with a high tilt-angle (almost 45°) showing the first order SmC* to N* phase transition. If strong anchoring is assumed, on the cell electrodes the molecules are aligned within the plane of the electrode and deviate from the cell plane in the bulk. The smectic layers are perpendicular to the cell surfaces and the angle between the layers normal and the rubbed axis is approximately equal to 45°. The projection of molecules, on a plane parallel to the cell surfaces, rotate by an angle close to 90° from one electrode to other and the ferroelectric polarization by an angle close to 180° [14]. So, the particular orientations of the director on both surfaces produce a helical structure with a helical axis perpendicular to the glass plates; the helical pitch is then equal to four times the cell thickness. The cell is placed between crossed or parallel polarizers. These cells give also a V-shape electro-optical response [13]. Our previous studies of these type of cells [14–15] have shown that a weak polarisation allows the development of a regular twisted structure in the whole bulk (wave guide regime), whereas a high spontaneous polarisation of molecules forces the director to be aligned in the bulk (“block polarisation” model [8]); so that the twists are throw back to the surfaces [8,13]. The effect of an applied voltage to the cell will be then to turn the molecules around their smectic cone, so the SmC* liquid crystal acts as a birefringent plate in the middle of the cell and as a rotator close to the surfaces, producing a V-shape electro-optical response [14]. Experimental studies are generally in good agreement with these interpretations. Recently we show that the observed widening of the V-shape transmission curves is related to the alignments layers thicknesses that separate the conducting electrodes from the liquid crystal in the cell [8,12,16]. It remains however some points to clarify such as the asymmetry and the shift of the V-shape transmission curves observed sometimes. It is generally accepted that the ionic charges are partly responsible for the shift leading sometimes to an asymmetry of the transmission curves [10]. When a twisted cell is filled with a SmC* liquid crystal with a high spontaneous polarisation, the divergences of \vec{P} produces polarisation charges which give rise to an electric field which is localised near the surfaces [8,14]. Even if any voltage is applied to the cell, the ionic charges originate from impurities naturally present in the liquid crystal compound moves in order to counteract the polarisation electric field. As consequence, an inhomogeneous initial repartition of the ionic charges must be present in twisted cells [16], whereas in classical SSFLC cells this repartition

is homogeneous. So, studies of the TSC optical transmission are particular since the ionic field exists even if any external field is applied to the cell. When an electric field is applied to this cell, the liquid crystal director reorients and the ionic impurities redistribute in the cell, so it's important to take into account the ionic field which tend to oppose to applied electric fields effects.

In this work, the main attention is directed on the studies of the ionic charges when an external field of a given frequency is applied to the TSC cell. Experimental studies show that the V-shape profile is affected by the ionic field. The internal electric field which takes into account polarisation and ionic charges contributions is given. Numerical results show how the ionic charges distribution in the cell influences the director orientations. Our studies explain firstly how the azimuthal angle distribution is modified in the presence and in the lack of ions impurities in the cell and secondly how the transmitted light intensity is affected. The reported numerical and experimental results agree well.

2. THEORETICAL STUDIES

2.1. Theoretical Model

Calculation of the transmitted light by TSC cells requires the knowledge of the azimuthal angle distribution through the cell. The symmetry of the problem suggests that the internal electric field $E(z,t)$ and the azimuthal angle $\varphi(z,t)$ are only time and z -dependants [16]. The z -axis is perpendicular to the electrodes of the cell. To obtain $\varphi(z,t)$ distribution, we follow Nakagawa *et al.* and Anabuki *et al.* [17–18] by minimizing the total free energy which is the sum of the dielectric energy, the elastic one, and the interaction energies between the internal field and both the spontaneous polarisation vector of the material and the net charge $n(z)$. Let us recall that the internal electric field is the sum of the applied field, the polarization and the ionic one. The minimization of the total free energy leads to the Euler-Lagrange equations which describe the elastic and electric (Poisson equation) properties of the cell. The liquid crystal reorientation is described by the following equation:

$$\gamma \cdot \frac{\partial \varphi(z,t)}{\partial t} = A \left(\frac{\partial^2 \varphi(z,t)}{\partial z^2} \right) - P_S \cdot \sin \varphi(z,t) \cdot E(z,t) \quad (1)$$

Where γ is the effective rotational viscosity coefficient, $A = K \sin^2 \theta$ where K is the elastic constant (in the one elastic constant approximation) and θ the smectic tilt angle and $E(z,t)$ is the internal electric field.

In order to obtain an expression of the internal effective electric field, we developed the Poisson's equation in the same way as Scaler-andi *et al.* and Maximus *et al.* [19–20]. The internal electric field is then given by:

$$E(z, t) = \beta \left[-\frac{V_0}{d} + \frac{P_S}{\varepsilon_{\perp} d} \int_0^d \cos(\phi(z, t)) dz - \frac{1}{d} \int_0^d e_i(z, t) dz \right] + e_i(z, t) - \frac{P_S}{\varepsilon_{\perp}} \cos(\phi(z, t)) \quad (2)$$

Where $e_i(z, t)$ is the ionic field in the z position: $e_i(z, t) = \frac{q}{\varepsilon_{\perp}} \int_0^z n(z, t) dz$ and $n(z, t) = n_+(z, t) - n_-(z, t)$ where $n_+(z, t)$ and $n_-(z, t)$ are the density of the positive and negative ionic charges respectively. The coefficient β depends on the cell and the alignment layers thicknesses (d and λ_{al}) and the dielectric permittivity of the liquid crystal (ε_{\perp}) and the alignment layer one (ε_{al}): $\beta^{-1} = 1 + \frac{2\varepsilon_{\perp} \cdot \lambda_{al}}{d \cdot \varepsilon_{al}}$ if both alignment layers thicknesses are equal and $\beta = 1$ if the alignment layers thicknesses are neglected. Here the anisotropy of the dielectric permittivity is neglected, so $\varepsilon_{\perp} = \varepsilon_0 \varepsilon_r$.

In the Eq. (2), V_0 represents the applied voltage to the cell by the power supplier, d is the liquid crystal thickness, the term $\beta \frac{P_S}{\varepsilon_{\perp} d} \int_0^d \cos(\phi(z, t)) dz - \frac{P_S}{\varepsilon_{\perp}} \cos(\phi(z, t))$ is the resultant field of the polarisation charges repartition. The last contribution to the internal field is $-\frac{\beta}{d} \int_0^d e_i(z, t) dz + e_i(z, t)$ which is related to the ionic charges repartition.

The motion of ions impurities will be described by the following equation [7,18,19]:

$$\frac{\partial n_{\pm}}{\partial t} = \frac{\partial}{\partial z} \left[\mp \mu_{\pm} n_{\pm} E + D_{\pm} \frac{\partial n_{\pm}}{\partial z} \right] \quad (3)$$

Where μ_{\pm} is the mobility of the positive or negative ions and D_{\pm} the corresponding diffusion constant: $D_{\pm} = \mu_{\pm} k_B T / q$ (k_B is the Boltzmann constant).

The last equation will be solved by considering that the number of the two ions species is constant in the cell and the current vanishes on the cell boundaries ($z = 0$) and ($z = d$):

$$J_{\pm}(z, t) = q \left[-\mu_{\pm} n_{\pm} E(z, t) \pm D_{\pm} \frac{\partial n_{\pm}}{\partial z} \right] = 0, \quad \text{for } z = 0 \text{ and } z = d. \quad (4)$$

The migration of ions in the cell is related to the applied voltage. In the classical SSFLC cells, the repartition of ionic impurities at the first step of the calculus $n_{\pm}(z, t = 0)$ is homogenous. On the other hand, the situation is quite different in TSC cells. Indeed, the main particularity

TABLE 1 Values of the Physical Constants used in our Calculations

μ_{\pm} (Ionic mobility)	$10^{-12} \text{ m}^2/\text{Vs}$
n_{\pm} (Ionic density)	2.10^{21} m^{-3}
D_{\pm} (Diffusion coefficient of the two species of ions)	$25.10^{-15} \text{ m}^2/\text{s}$
P_S (Spontaneous polarization)	72 nC.cm^{-2}
A (Elastic constant)	8.10^{-11} N
ϵ_{CL} (Dielectric permittivity of the liquid crystal)	13
ϵ_{AL} (Dielectric permittivity the alignment layer)	4
γ (Viscosity)	3 Pa.s

of these cells is the presence of a natural internal electric field due to the polarisation charges even if no voltage is applied to the cell. Therefore, ions must migrate in the media to counteract this internal field; and the consequence is that the ionic impurities repartition before applying any voltage is not homogeneous. Thus when an external voltage will be applied to a TSC cell, the ions migration will be quite different in comparison with classical SSFLC cells.

Equations (1), (2) and (3) will be used to study the dynamical properties of the TSC cell when an external electric field of frequency f is applied to this cell. The azimuthal angle distribution of the director will be modified as well as the transmitted intensity. According to the applied electric field frequency, the ionic charges distribution and then the ionic field in the cell will be more or less influenced. Equations (1), (2) and (3) will be solved numerically by using the initial conditions (4) and assuming hard anchoring (i.e. $\varphi(0, t) = 0$ and $\varphi(d, t) = \pi$). In order to simplify the problem, we consider that the cell contain the same number of positive and negative ions. We consider also that the negative and positive ions have the same diffusion coefficient and mobility. The precedent set of equations were solved with the following values (see Table 1).

2.2. Results and Discussions

Let us start by giving some results for a frequency $f = 10 \text{ Hz}$ and when the ionic impurities effects are neglected (Figs. 1 and 2). For lower applied voltages (almost -4 Volts), the azimuthal angle is weak in practically all the cell except close to the upper surface where it varies abruptly to reach 180° . The transmitted light intensity reaches a maximum. When the applied voltage is increased, the spontaneous polarization aligns gradually with the total electric field and the azimuthal angle distribution and the transmitted light intensity change. When this intensity reaches a minimum, the curve of the azimuthal angle distribution is practically symmetrical with respect to the center

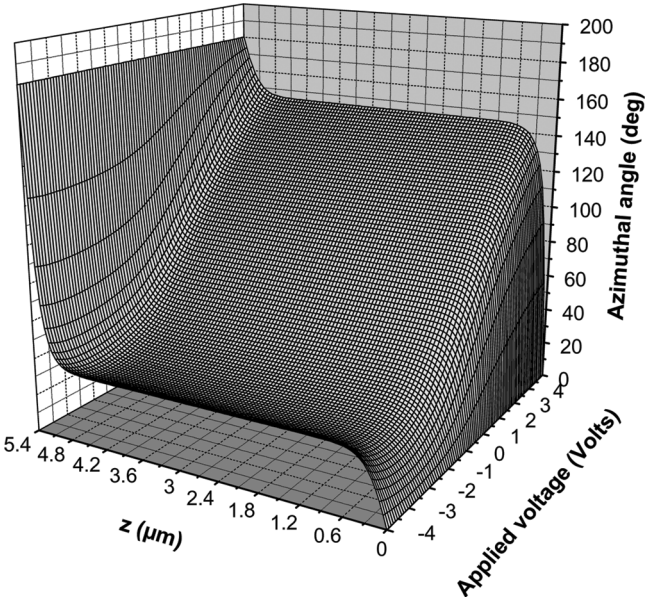


FIGURE 1 Azimuthal angle distribution in the absence of ion impurities.

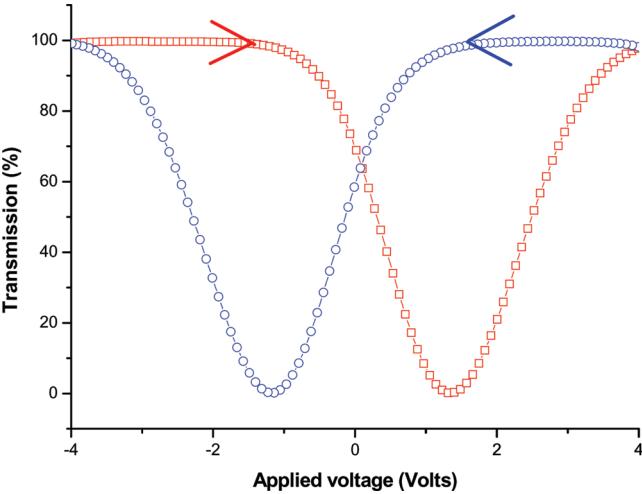


FIGURE 2 Transmitted light intensity in the absence of ion impurities. The observed hysteresis is due to the viscosity effect.

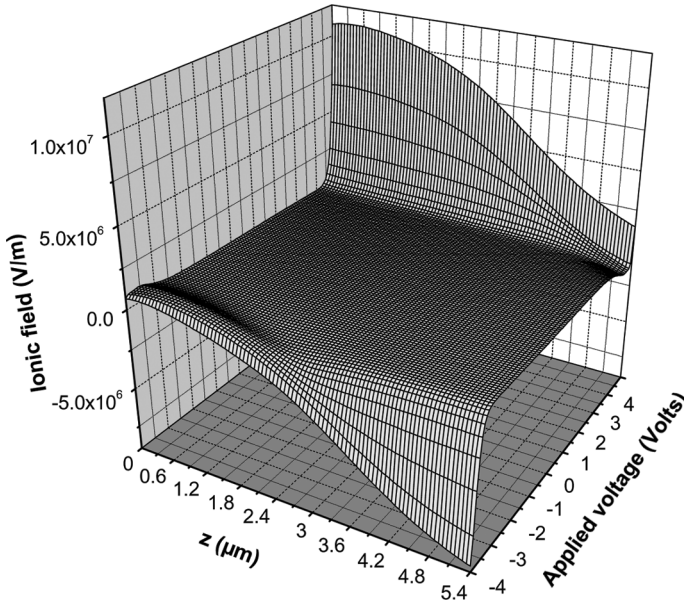


FIGURE 3 Ionic field in the TSC cell calculated for the ionic impurities density $n_{\pm} = 2 \cdot 10^{21} \text{m}^{-3}$.

of the cell. By increasing the applied voltage, strong twists of the director are rejected towards the lower parts of the cell and the intensity increases to reach the plate which corresponds to its maximum. We should mention that the shift of the minimum of the transmitted light intensity with respect to the zero of the applied voltage increases with frequency.

Figure 3 shows the calculated ionic field for ionic impurities density $n_{\pm} = 2 \cdot 10^{21} \text{m}^{-3}$ and viscosity $\gamma = 3 \text{Pa} \cdot \text{s}$. When no voltage is applied to the cell, the azimuthal angle distribution is not constant. So, the ionic impurities are not homogeneous and the ionic field exists in the cell (Fig. 3). As result, the twists are less strong in the cell (Fig. 4). When a voltage is applied to the cell, except near the cell surfaces where the ionic field varies abruptly, this field remains almost constant everywhere else in the cell. The cell acts as if a constant field is added or subtracted to the applied one. What results in one hand on smoothing the azimuthal angle distribution and the transmitted light intensity and on the other hand on a shift and a deformation of the transmission curve in comparison with the curve obtained when the ionic impurities are not considered (Figs. 1 and 6).

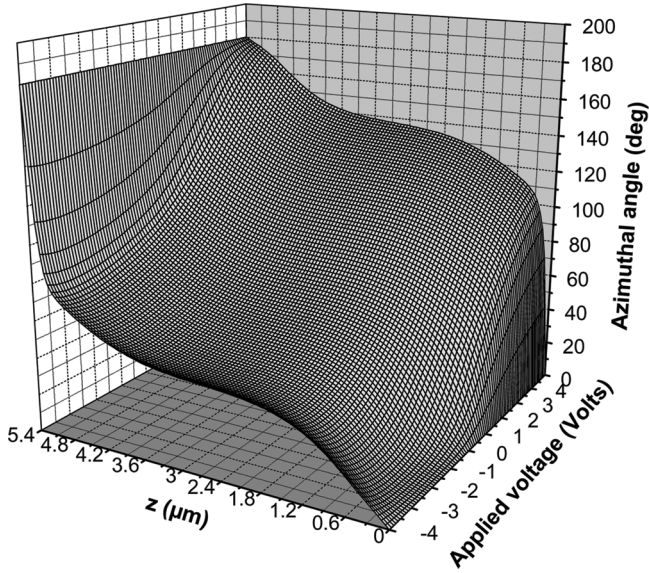


FIGURE 4 Azimuthal angle distribution calculated for ionic impurities density $n_{\pm} = 2 \cdot 10^{21} \text{m}^{-3}$. The twists are less abrupt in the cell.

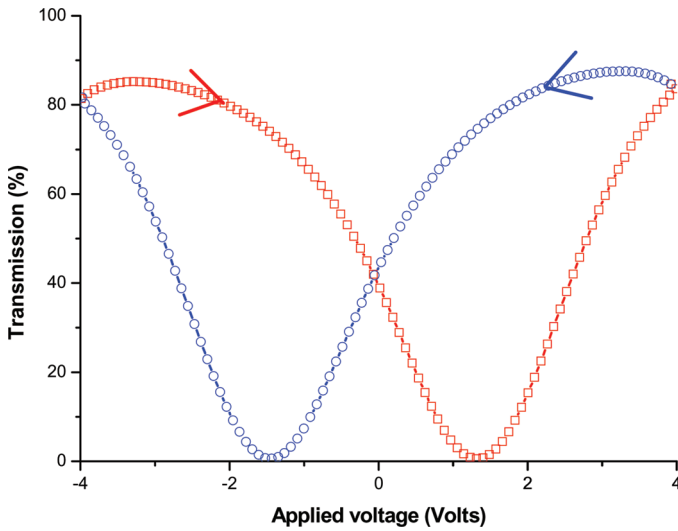


FIGURE 5 Transmitted light intensity calculated for ionic impurities density $n_{\pm} = 2 \cdot 10^{21} \text{m}^{-3}$. The observed hysteresis is related to the viscosity and ionic impurities effects.

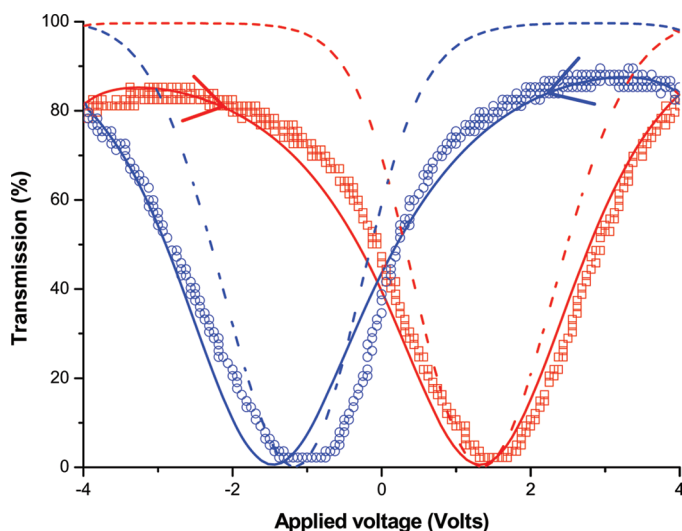


FIGURE 6 Transmitted light intensity curve obtained when applying a triangular wave of frequency $f = 10$ Hz. Experimental curves (circle and rectangle). Calculated curves: discontinued line (cell without ion impurities), continued line (cell with ion impurities).

3. EXPERIMENTAL STUDIES

The rubbing directions of the electrodes of the studied cell are perpendicular to each other. The thickness of the cell is equal to $5.4 \mu\text{m}$. The cell is filled with a SmC* liquid crystal (CS2005 – from Chisso). This compound possesses high tilt-angle (almost 43°) which is almost temperature independent. A strong anchoring is assumed so, the molecules are co-planar on the cell electrodes and deviate from the cell plane in the bulk. The smectic layers are perpendicular to the cell surfaces and the angle between the layers normal and the rubbed axis is approximately equal to 45° . From one electrode to other, the polarization vector of the ferroelectric rotate by an angle close to 180° . The cell is put between parallel polarizers and illuminated by a HeNe laser ($\lambda = 632.8 \text{ nm}$). The transmission of the normally incident polarized light through the cell and the analyzer was monitored with a photodiode and a HP54645A digitizing oscilloscope. A triangular voltage is applied to cell by using an HP33120A function generator. The entrance polarizer is aligned parallel to the analyzer and the cell is placed in such a way that the transmitted light intensity reaches a maximum when a sufficient voltage is applied to the cell. All measurements were carried out at room temperature.

Figure 6 shows the experimental transmission curves (square and circle) when applying a triangular wave of frequency $f = 10$ Hz and the theoretical ones obtained first in the case where the ionic impurities are not considered (discontinued line) and then accounted for (continued line). The arrow indicates the direction of variation of the applied voltage. Both electro-optical response curves resemble to a deformed V letter and show the existence of threshold and hysteresis. This type of response was already reported in the literature and was referenced as “W-shape” [21]. However the curve corresponding to the increase of the applied voltage differs slightly from the one which corresponds to a decrease of the applied voltage. It is well known that these behaviours are related to the alignment layers, the viscosity of the material and the ionic charges present in the cell [21]. It's well established that the alignment layers controls also the widening of the transmission curves [16]. Consequently, the thicknesses of the alignment layers are found to be equal to 40 nm. On the other hand, it's well known that the viscosity effect appears more at high frequencies and the ions impurities effect at low frequencies. The theoretical curves calculated without considering the ionic impurities do not correspond at all to the experimental one. However curves obtained by considering the ionic impurities of density 2.10^{21} m^{-3} agree well with the experimental curves. At the frequency $f = 10$ Hz, the ionic charges have no more time to move under the applied electric field in order to counteract its effects. They remain localized at same place of the cell and the ionic field does not vary and acts only close to surfaces (see Fig. 3). The applied electric field is then used to reorient the liquid crystal and to eliminate the ionic electric field effect. As a result, when ion impurities are present in the TSC cell, the azimuthal angle distribution and the transmission curve are modified. The observed asymmetry in the experimental curves is probably related to the presence of several ionic species in the cell and to their mobility differences.

4. CONCLUSION

We study the electro-optical behaviour of twisted SmC* cell with high spontaneous polarization which is known to exhibit a V-shape like switching profile. We show that the viscosity and the ionic impurities modify the electro-optical response. The viscosity effect amounts to the shift of the minimum of the transmitted light intensity with respect to the zero of the applied voltage. The ionic impurities act in the TSC cell even if any field is applied to the cell. Their distribution is inhomogeneous and the ionic field always exists in the cell. In this case, the effect of the polarization charges can be totally canceled by the

presence of ions impurities, the cell behaves then like if the polarization charges are neglected [13]. As result, the twists are less strong in comparison with the case where the ionic impurities are not considered. For the case of the applied voltage considered in this study, the cell acts as if a constant field is added or subtracted to the applied one. The azimuthal angle distribution and the transmitted light intensity curves become smooth. A shift and a deformation of the transmission curve is observed in comparison with the one obtained when the ionic impurities effect is not considered. The experimental studies confirm the observed behaviors.

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