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Influence of the Ion Mobility on the Exact Location of the Regime Bump in NLCDs

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Influence of the Ion Mobility on the Exact Location of the Regime Bump in NLCDs

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In this article, we propose an improvement of the ion transport model in NLCDs, taking into consideration the possible dependence of the ion mobility on the ion density. The presence of ion channels in the LC bulk, initiated by a Carr-Helfrich-like mechanism, would lead to a higher mobility at the start of the regime pulse. A better explanation of the exact location of the current bump during the regime pulse can then be reached.

Keywords: transmissive NLCDs; ion transport; convective instabilities

INTRODUCTION

Nematic Liquid Crystal Displays occupy an important part of the exploding Flat Panel Display market. However, the existence of ion impurities in the displays disturbs a lot their electro-optical properties and causes them to deteriorate. A correct understanding of the ion effects in the liquid crystal bulk is therefore necessary.

Our group has contributed to this work by defining ion transport equations and by developing an adequate simulation program [1].

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Experimental studies have also been performed using the transient method. This method consists in measuring the ion current in prototype cells driven by a square wave voltage (SQW) below threshold. The first pulse gives the transient current from which can be deduced the density of ions in motion in the LC, their mobility and their transit time (time necessary to cross the thickness of LC bulk) [2]. The next pulses give the regime currents. Our simulation program allows a good reproduction of the measured transient results. However, the regime currents exhibit a bump. An exact simulation of this behaviour has always been a problem. A macroscopic model describing the trapping of ions at the alignment layers was proposed [3]. The reconstitution of the bump in the simulation was possible but it came too late compared to the measured one.

In the following, we propose to take into account a new element in our ion transport theory that brings a nice simulation of the regime current : a brutal change in ion mobility, at the start of each regime pulse. Our proposal is inspired from the observation in many nematics of electrohydrodynamic instabilities giving Williams-domains in the low frequency range [4].

TRAPPING AND RELEASE EFFECTS

In the LC-bulk, the transport properties of each ion specie with density n_i (m^{-3}) are determined by drift and diffusion processes. The equation of motion can be written as (one-dimensional case):

$$\frac{\partial J_i}{\partial z}(z,t) = \mp e \frac{\partial n_i^{\pm}(z,t)}{\partial t} = \frac{\partial}{\partial z}(\mu_i(z).n_i^{\pm}(z,t).E(z,t)) \mp \frac{\partial^2 D_i(z).n_i(z,t)}{\partial z^2} \qquad (1)$$

$J_i(z,t)$ (A/m^2) is the current density contribution caused by positive and negative ions of type i at a distance z in the liquid crystal. The diffusion constant D_i is related to the mobility μ_i by the Einstein's relation $D_i / \mu_i = k.T / e$ (with k the Boltzmann constant, e the elementary charge and T the temperature). Measurements have shown that many ions are actually trapped at the alignment layers for some time before they are transported to the other side. In the past, Maximus and Colpaert [3] postulated a clear model for the ion trapping during the regime current.

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They based their model on the findings of Vaxiviere, Yamashita, and Yanagisawa [4,5,6]. This adsorption and desorption model is given by the analytical expression (with a = 0 or d_{LC}):

$$J_i^{\pm}(a,t) = -e\frac{\partial N_{trapped}^{i,top}(t)}{\partial t} = e\left(\frac{N_{trapped}^{i}}{\tau_{trap}^{i}} - k_{trap}^{i} n^{i}(a,t)\right) \qquad (2)$$

The ions are caught with a trapping constant k_{tr} (order of 1e-7m/s) and released with a release time τ_{tr} (smaller than the transit time). k_{tr} and τ_{tr} must be scaled with the voltage which indicates that they originate from an electrical process near the alignment layers (als) [7].

An example of transient and first regime currents measured and simulated is given in Figure 1 for a transmissive cell with low mobile ion density. The 8μm TN-cell is filled with ZLI-4757 (with $\Delta\varepsilon$=0.6, V_{10}=5.75V, V_{app}=4V and f=1Hz). The transient current decreases linearly piece by piece revealing the presence of two main ion species, the first one with mobility six times higher than the second one. Since a short circuit period is preceding the measurements, the ion distribution is always homogeneous at t=0s. The amount of trapped ions during the transient pulse is thus negligible and no bump exists. At the start of the second pulse $t=t_1$=0.5s, most of the ions are next to the als. That causes an important trapping phenomenon, which becomes visible in the current profile by the

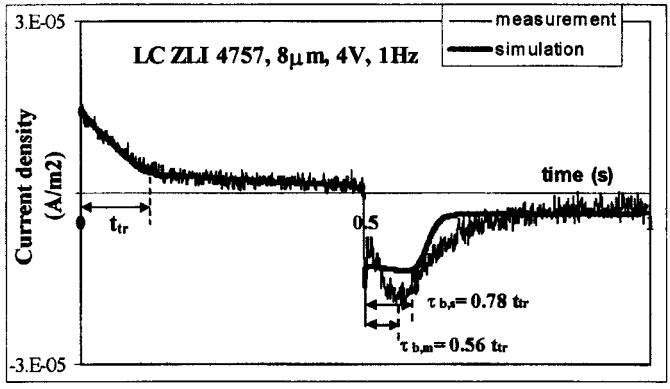

FIGURE 1 Measurement versus simulation: $n_1=9e^{17}/m^3$, $\mu_1=1.32e^{-10}$ m^2/Vs; t_{tr}=0.12s, $n_2=2e^{18}/m^3$, $\mu_2=2.26e^{-11}m^2/Vs$.

intermediate of the bump. The time at which the bump appears is denoted τ_b. The increase of the current before τ_b is caused by the release of ions from the alignment layers while the decrease afterwards is due to the first arrivals of ions at the other side.

Because of the diffusion force, the regime bump comes earlier than the transit time ($\tau_b < t_1$). At the start of the regime pulse t_1, the ion velocity is effectively risen by the high ion density gradient next to the alignment layers (no more homogeneous distribution, see equation 1). The measured bump time τ_b is at about 50% (or even less) of the transit time t_{tr}. However, the simulations show a higher τ_b value: around 70 % of t_{tr}. Moreover, the measured current profile has a much higher regime peak than the simulated one. These differences can be explained by a real acceleration of ion motion at the start of regime, more important than the one introduced in our simulations by diffusion and drift processes.

IMPROVEMENT OF THE BUMP MODEL

To solve the ion bump problem numerous solutions were proposed. Generation and recombination processes were studied. They always led to unsuitable results, the current keeping on increasing from one regime pulse to the other [8, 9]. We also tried to explain the time difference between experiment and theory studying the influence of the second ion kind mobility on the regime current profile. If the transient time t_1 is chosen shorter than the transit time of the second ion kind, this slower ion kind will not separate completely at the end of the transient pulse and the speed increase created during the second pulse by the diffusion/trapping phenomenon will be lessened. This improvement only enables the simulated bump time τ_b to come 1% or 2% earlier. The effect can be enhanced adding more ions. But, this enlarges the current bump since in that case the second ion kind is showing its own bump at $\tau_{b2} > \tau_{b1}$. If the mobility of the slowest ions was less high, the effect could also be increased but in that case the symmetry between positive and negative regime currents would be lost. The second ion specie can't bring a good correspondence between the measured and the simulated current bumps.

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We have then carried out a new assumption based on the theoretical consideration of the presence of Williams-like Domains in the bulk within a short period after the voltage reversal.

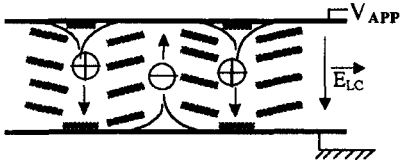

FIGURE 2 Formation of Williams-like domains.

The Williams domains correspond to a regular pattern of bright and dark stripes perpendicular to the director long axis [10,11]. In that configuration, the molecules are periodically distorted. Their distribution "in layers" is due to an important ion flow across the LC-bulk.

Their origin is the two-dimensional Carr-Helfrich effect involving positive and negative ions which move throughout the LC in separate channels (Figure 2) [12]. In the conduction regime (Low Frequency Limit), the molecules configuration remains the same while the ion motion follows the AC-field. The threshold voltage of the domains can be low and the molecular spatial period in the order of the cell thickness. Recently, Ochi investigated domains in 5CB cells ($\Delta\varepsilon$ =10) corresponding to transient herringbone patterns [13]. He has noticed that these domains appear when the ions transit from one electrode to the other during the regime period. He showed that the maximum in intensity of the ring and stripe-like patterns coincides with the maximum in the ion current (caused by the parallel mobility). His study confirms the narrow relationship between the deformation of the LC structure and the ion motion throughout the LC bulk

DEPENDANCE OF THE MOBILITY ON THE ION DENSITY

The Carr-Helfrich mechanism giving the Williams-like domains is a possible solution to our current bump issue. One necessary condition to get domains is to have a conductance anisotropy; our cells exhibit an important one ($\sigma_{//}/\sigma_{\perp}$ =1.8). Homogeneous LC materials with positive dielectric anisotropy and sufficiently small $\Delta\varepsilon$ can very likely have domains below the

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Frederiks transition [4]. We can reasonably consider that our cells respects this condition ($\Delta\varepsilon$=0.6). The estimation of the critical frequency below which the domains are stable is 26Hz and is much larger than the used 1Hz AC-field frequency [4].

If the ions are moving in channels, it seems possible that their actual mobility will be no longer determined by the mobility perpendicular to the molecules but also by the one parallel, provided that a sufficient amount of ions are in motion in the LC-bulk. A new formula for the mobility has then been introduced in our one-dimension simulation program (equation (4), θ is the tilt angle, $\Delta\mu=\mu_{\perp}-\mu_{//}$ is the mobility anisotropy).

$$\mu(z) = \mu_{\perp}\cos^2(\theta) + \mu_{//}\sin^2(\theta) + (\Delta\mu)\cos^2(\theta)\left[\frac{1}{2} + \frac{1}{2}\tanh\left(\frac{\sum_i n_i(z) - n_{thres}}{n_{ref}}\right)\right] \quad (4)$$

The first two terms are the ones used in the original simulations; they give the mobility variation in case of molecular switching. The third one is an empirical expression describing the possible mobility increase due to the formation of ion channels below the Frederiks transition. The change in mobility is subjected to two parameters: the threshold density n_{thres} and the reference density n_{ref}. When the ion density is below n_{thres}, no molecular redistribution (created by a strong ion flow) and then no change in mobility can intervene. This is the case during the transient pulse. A reasonable value for n_{thres} is given by the space charge limit related to the LC Frederiks transition (SCL =1.25e^{19} m^{-3}), which is higher than the transient density. As for n_{ref}, it indicates the sharpness of the variation from $\mu_{\perp}$ to $\mu_{//}$ versus the ion density value. n_{ref} must cause a brutal change in mobility to keep the ion mobility always constant during the transient pulse and thus to avoid deformation of the simulated transient current.

At the start of the regime pulse, the local ion density next to the als is: $(eV_{app}/kT).n_{tran}$, which exceeds n_{thres}. Consequently, with an ion density below n_{thres} for transient and above for regime, the regime mobility is $\Delta\mu$ higher than the transient mobility. The new formula (4) can give rise to anomalies in the simulated current profile (just after the reversal of the voltage and at the arrival of the fastest ion kind next to the alignment layers). These anomalies don't appear anymore considering that the domains can't be reasonably formed at the borders but only in the LC-bulk. The

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anchoring forces prevent indeed the formation of these domains. The resulting current simulation is shown in Figure 3, which provides a much nicer fit between theory and measurement is obtained. The fact that higher acceleration process occurs just after the voltage reversal in the new model has also ameliorated the simulated bump shape and the height of the regime peak (the simulated bump without domains was indeed not high enough and too flat before τ_b).

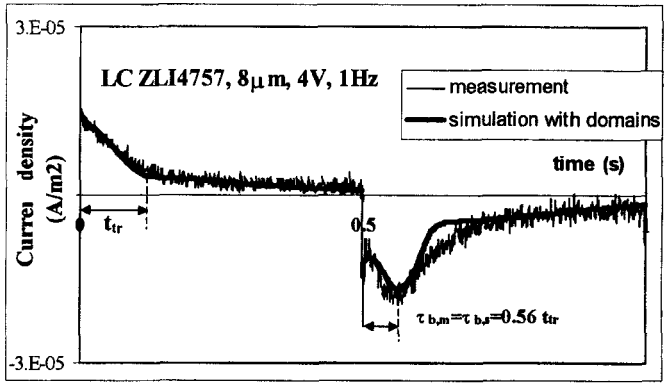

FIGURE 3 Measurement versus simulation with domains, $n_{thres}=1.25e^{19}/m^3$; $t_{tr} = 0.12s$, $\tau_{b,m} = \tau_{b,s} = 0.57\ t_{tr}$.

CONCLUSION

We have studied ion transport properties in nematic transmissive cells. The bump present in the simulated regime current profile appears too late compared to the measured one. The introduction of a change in ion mobility at the start of the regime pulse in our simulation program has permitted a better fit with the experimental observations. The mobility increase would be caused by the creation of Williams-Like domains in the LC bulk. A threshold density equal to the Frederiks SCL must be exceeded to initiate the phenomenon, which exists only at the start of the regime pulse.

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In the future it will be important to valid our model with further experimental studies. In particular the temperature and the time dependency of the bump time with the ion density can bring precious information. The optical observation of the domains would be interesting but difficult to perform because of the rather small director deviations when applying sub-threshold voltages. The study of ion transport in two and three dimensions will be necessary to get more insight in this model.

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