

Two-dimensional Monte Carlo based Ion Transport algorithm in Liquid Crystals.

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ABSTRACT

In liquid crystal devices (LCD) where the electrode structure has a microscopic pattern, as in In-Plan-Switching (IPS) or multi-domain Vertically Aligned Nematic (VAN), ion transport in two dimensions is relevant.

In this paper we propose a new Monte Carlo based 2D algorithm to calculate ionic transport in Liquid Crystal Devices.

INTRODUCTION

Most liquid crystal (LC) materials contain ions with concentrations in the order of 10^{16} - 10^{21} per m^3 . Even when the concentration seems relatively low, the ions can have an important influence on the electrical field and the director orientation in the LC. The simulation of ion transport in LC is essential to understand and estimate these influences.

In LC devices where the electrode structure has a microscopic lateral pattern, as in In-Plan-Switching (IPS) or multi-domain Vertically Aligned Nematic (VAN) devices, ion transport in two dimensions is relevant.

In this paper we propose a new Monte Carlo based 2D algorithm to calculate ionic transport. This algorithm has been developed to decrease calculation time, by avoiding small position and time intervals as used in finite-element and finite-difference methods.

THEORY

The Monte Carlo based 2D-ion transport algorithm calculates the new position of "meta-ions" using the principles of drift and diffusion. A meta-ion is an object, which represents a large number of ions. This is used to reduce calculation time.

$$r_i(t + \Delta t) = r_i(t) + \bar{\mu} \cdot E \Delta t + \Delta r_{diffusion} \quad (1)$$

Formula (1) is the transport equation of meta-ion i . The position of meta-ion i at time $t + \Delta t$ is the position at time t plus a change in position due to drift and diffusion. The drift term is straightforward. It is the product of the mobility tensor and the local electrical field vector, multiplied with time step Δt ($\bar{\mu} \cdot E \Delta t$).

Thermal diffusion is calculated as a random displacement, with a Gaussian distribution, which takes into account the anisotropy and the orientation of the director in the LC-material. First the random displacement is calculated in the coordinate system where the director is parallel with the z-axis. We assume Gaussian distributions parallel with the LC director with $\sigma_{||}^2 = 2D_{||}\Delta t$, and in the perpendicular directions with $\sigma_{\perp}^2 = 2D_{\perp}\Delta t$. After the randomly chosen displacement in three dimensions, a rotational transformation is performed to transform the coordinates to the LC coordinate system. In this 2-dimensional LC coordinate system only the z and y coordinate are important

It is obvious that formula (1) can only be applied to the transport of meta-ions in the bulk of the material. Near the interface ions tend to pile up in an exponential distribution. This can be found from the steady state solution of the one-dimensional differential equation [1] given by formula (2).

$$\frac{\partial n^{\pm}}{\partial t} = \mp \mu_{zz} \cdot \frac{\partial}{\partial z} (n^{\pm} \cdot E_z) + D_{zz} \cdot \frac{\partial^2 n^{\pm}}{\partial z^2} \quad (2)$$

Where n^{\pm} indicates the concentration of positive and negative ions, respectively, and D_{zz} is the diffusion coefficient in the z direction. If we set the left-hand side of (2) equal to zero for steady state, we obtain formula (3):

$$n^{\pm} = n_0^{\pm} \cdot e^{-\frac{eE_z}{kT} z} \quad (3)$$

With E_z the electric field at the interface, n_0 the ion concentration at the interface, z the distance from the interface and T the temperature.

We define 3 different regimes [2] for the calculation of the ion transport. The first one is the bulk regime where equation (1) holds without limitations. The second is near the interface when an electrical field is present. In this case formula (3) predicts a steady state exponential distribution perpendicular to the interface (z-direction). The last regime is when the ion is very close to the interface and when the electrical field is sufficiently weak. In this case only diffusion from the interface is important.

In this algorithm space is not discretized, and the meta-ions move in a rectangular continuum. With this algorithm, large time steps can be taken which leads to an important decrease in calculation times.

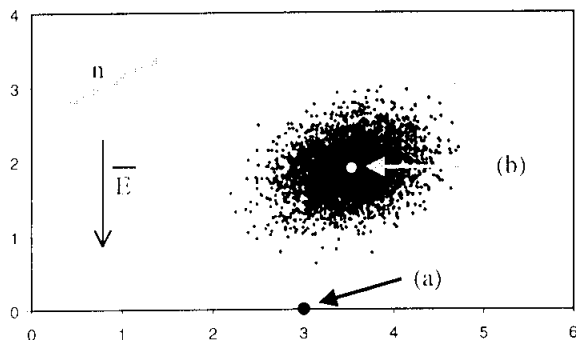


Figure 1: Distribution of 6000 negative meta-ions after simulating the transport in an anisotropic, homogeneous medium. With n : director orientation, E : electric field, a: start position, b: average position after 30 ms.

RESULTS

Testing the accuracy of this algorithm was performed by calculating the transport of meta-ions with an initial δ -distribution near the interface of an LCD. A constant electrical field in the z-direction was assumed and the director had a constant orientation, $\varphi_{\text{twist}} = 90^\circ$, $\theta_{\text{tilt}} = 30^\circ$. Figure 1 shows the positions of a number of meta-ions after 30 ms, after 20 time steps have been taken, together with the starting position of the δ -distribution (a). Position (b) is the average position of all meta-ions after 30 ms. The displacement between a and b is not parallel with the field, because of the anisotropy of the medium. The elliptical spreading around (b) is due to Gaussian diffusion under influence of the anisotropy and the director orientation of the LC-material. The scales are in μm ; n and E represent respectively the director orientation and the electrical field vector. E is 10^6 V/m. The perpendicular ion mobility is 5×10^{-11} m^2/Vs , the ratio $\mu_{\parallel}/\mu_{\perp}$ is 1.8.

As an example we consider the movement of meta-ions representing a small ion concentration in an IPS-structure. Figure 2 shows the equi-potential lines after the liquid crystal director has reached an equilibrium distribution. The voltage to the left electrode applied is 2 V; the right one is grounded. The calculation structure is $4 \mu\text{m}$ by $45 \mu\text{m}$ and has periodical boundary conditions.

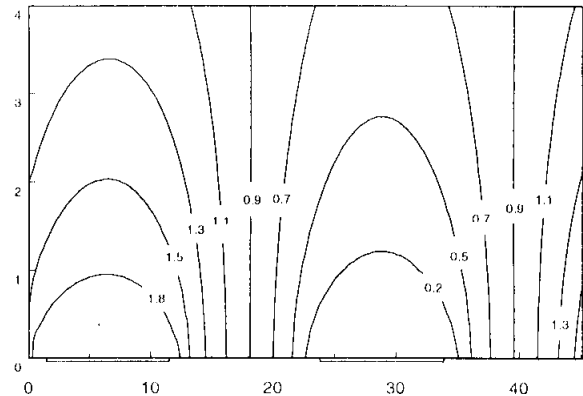


Figure 2: Equipotential lines in an IPS-structure. Unequal scales are labeled in μm , 2V applied. The grey rectangles represent the electrodes. The left electrode is at 2V, the right electrode at 0V.

At time $t = 0$ s we assume a homogeneous distribution of the meta-ions in the calculation structure. This can be experimentally achieved by short circuiting the LC cell for a longer period. The charge distribution is sufficiently low to assume that there is no influence of the ions on the potential distribution.

Figure 3 shows the sequence of 5 simulation results, every 100 ms, for positive meta-ions. The first distribution is at 100 ms, the last one at 500 ms, the time step is 10 ms. The perpendicular ion mobility is 5×10^{-11} m^2/Vs , the ratio $\mu_{\parallel}/\mu_{\perp}$ is 1.8.

First we discuss the behavior of these positive meta-ions in the first five hundred milliseconds. In the left half of the structure an upward electrical field repels the meta-ions from the positive electrode. The meta-ions are stopped by the presence of the upper glass substrate.

At the right side a downward electrical field attracts the meta-ions towards the negative electrode.

Figure 4 shows the simulation result after 5s (a) and 10s (b). Almost all positive meta-ions are gathered near the negative electrode. They have migrated, via diffusion and the small lateral component of the electrical field towards the

negative electrode. The time scale of this motion of the meta-ions is in the order of seconds.

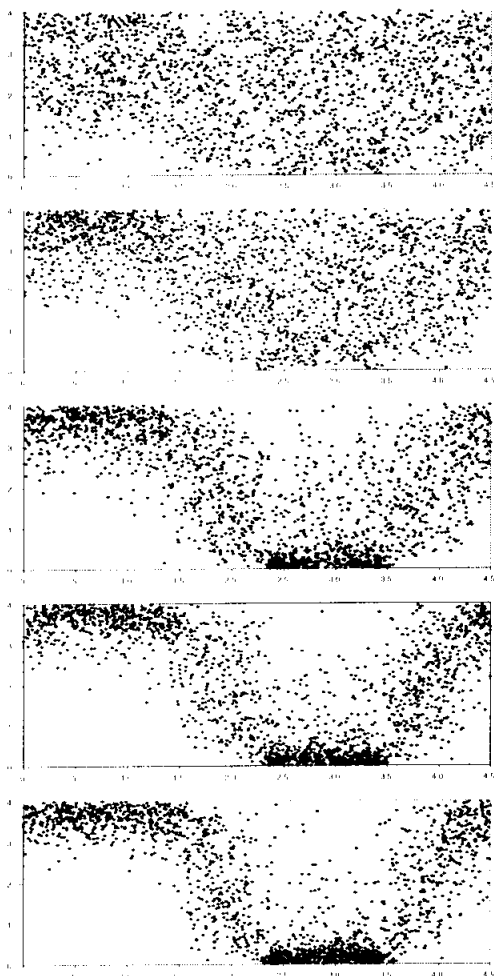


Figure 3 (a-e): A sequence of positive meta-ion distributions in an IPS-structure: 100 ms, 200 ms, 300 ms and 400 ms after starting with a homogeneous ion distribution.

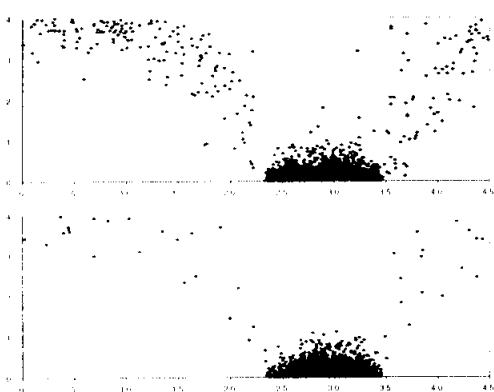


Figure 4 (a-b): Positive meta-ion distributions in an IPS structure: 5s and 10s after starting with a homogeneous distribution.

CONCLUSION

The proposed algorithm for simulating the transport of charged particles in LCD's yields reliable results. These ion transport simulations will be used in the future to determine the influence of the ions on the director orientation in the LC and on the optical transmission. The results are interesting because this 2D-ion transport algorithm can be used to study two-dimensional effects occurring in IPS cells or in pixels of an LC display.

REFERENCES

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