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Determination of nematic polar anchoring from retardation versus voltage measurements

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The popular “high-electric-field” technique to determine the polar anchoring coefficient W of a nematic–substrate interface requires the simultaneous measurement of the capacitance and optical phase retardation of a liquid crystal cell as a function of applied voltage. We develop a generalized model that makes it possible to eliminate the capacitance measurement. The new technique, called the RV (retardation versus voltage) technique, requires only the measurement of retardation as a function of applied voltage, and allows for the determination of W by a linear fit over a prescribed voltage window. The technique is not sensitive to uniformity of the cell thickness, does not require patterned electrodes, and allows for the local probe of the surface. The value of W obtained by the RV technique is the same as W obtained by the traditional technique. © 1999 American Institute of Physics. [S0003-6951(99)02828-4]

The surface orients a nematic liquid crystal director \mathbf{n} along a particular orientation, called “the easy axis.” External torques deviate \mathbf{n} from its easy axis. The energetic cost of this deviation is usually characterized by an anchoring coefficient W . A variety of techniques have been developed to determine W ,^{1–5} most of which test elastic deformations created by an external field. The most commonly used, especially for strongly anchoring cells of industrial interest, is the so-called “high-electric-field” (HEF) technique⁴ developed by Yokoyama and van Sprang.² It requires simultaneous measurements of the capacitance C and the optical phase retardation R of a nematic cell as a function of applied voltage V . W is determined by a simple linear fit of the data plotted in the form R vs $1/CV$ over some voltage window (V_{\min}, V_{\max}) which is well above the Frederiks threshold. The resulting W is only weakly dependent on the nematic bulk properties and does not require accurate knowledge of the cell thickness.

In this article, we seek to simplify the HEF technique by eliminating the measurement of the capacitance. The measurement of capacitance can be complicated since it requires patterned electrodes, as well as uniform cell thickness over a large area. Recently, Sun and Yokoyama suggested overcoming the difficulties by adding a small capacitance C_0 , in series with the liquid crystal cell and to approximate the dependence R vs $1/C-V$ by a dependence R vs $1/C_0V$.⁵ In this article, we analyze theoretically the response of the cell with a finite W to the applied field and show that this response can be completely characterized by the functional dependence R vs V without any additional capacitors in the circuit or any assumptions about the capacitance of the cell. This approach is made possible by deriving an equation for the cell capacitance as a function of applied voltage. Using

this equation in place of the measurement of capacitance, W can be determined by a simple linear fit of the experimental dependence R vs V . The experimental test for standard polyimide alignment agents produces the same value of W with and without the measurement of capacitance.

Theory: Consider a liquid crystal cell of thickness d confined between two electrodes at $z=0$ and $z=d$ (Fig. 1). When the electric field is zero, \mathbf{n} is oriented along the easy axis and makes an angle θ_p with the x axis. θ_p defines the minimum of the surface anchoring potential and is called the pretilt angle. In an external electric field, \mathbf{n} becomes z dependent and the free energy per unit area of the cell reads

$$F = \int_0^d \frac{1}{2} \left[(K_1 \cos^2 \phi + K_3 \sin^2 \phi) \left(\frac{d\phi}{dz} \right)^2 - \mathbf{D} \cdot \mathbf{E} \right] dz + 2 \left[\frac{1}{2} W \sin^2(\theta - \theta_p) \right], \quad (1)$$

where K_1 (K_3) is the splay (bend) elastic constant, $\mathbf{D} = \epsilon_0 \hat{\epsilon} \mathbf{E}$ is the electric displacement, $\hat{\epsilon}$ is the relative dielectric tensor, \mathbf{E} is the applied electric field (applied voltage $V = \int_0^d E_z dz$), ϕ is the angle between $\mathbf{n}(z)$ and x axis, and $\theta = \phi(z=0, d)$. The deviation $\theta - \theta_p$ is taken to be small so

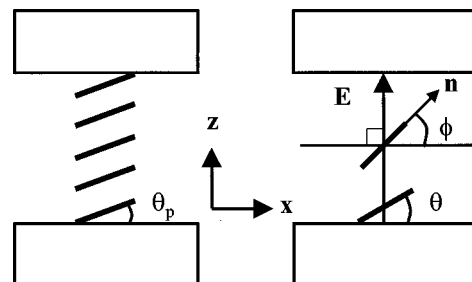


FIG. 1. Director configuration in the cell without field (left-hand side) and with an applied electric field (right-hand side).

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that the energetic cost of surface director deviations can be approximated by the Rapini–Papoular potential.⁶ Note that Eq. (1) neglects any possible effects of the divergence elastic K_{13} term in the free energy, and assumes that the effects of free electric charges are negligible. From the Maxwell equation $\text{div } \mathbf{D} = 0$, then, in a cell with a one-dimensional distortion, D_z does not depend on z . With this and the Euler–Lagrange equation, the applied voltage V , optical phase retardation R , and capacitance C are integral parametric functions with parameters $y_m = \sin^2 \phi_m$, where ϕ_m is the director angle at $z = d/2$, and $y_b = \sin^2 \theta$:

$$V = \frac{V_{th}}{\pi} \sqrt{1 + \gamma y_m} I_V(y_b, y_m), \quad (2)$$

$$R = \frac{2\pi dn_0 \nu}{\lambda} \frac{I_R(y_b, y_m)}{I_C(y_b, y_m)}, \quad (3)$$

$$C = \frac{\epsilon_0 \epsilon_{\perp} S}{d} \frac{I_C(y_b, y_m)}{I_V(y_b, y_m)}. \quad (4)$$

Here, ϵ_{\parallel} and ϵ_{\perp} are the components of the dielectric tensor that are parallel and perpendicular to the director, respectively, $\gamma = (\epsilon_{\parallel} - \epsilon_{\perp})/\epsilon_{\perp}$, $V_{th} = \pi \sqrt{K_1/\epsilon_0 \epsilon_a}$, $\epsilon_a = \epsilon_{\parallel} - \epsilon_{\perp}$, $\nu = (n_e^2 - n_o^2)/n_e^2$, n_o and n_e are ordinary and extraordinary refractive indices, respectively, S is the overlapping electrode area, λ is the wavelength of the probing light, and

$$I_V(y_b, y_m) = \int_{y_b}^{y_m} \sqrt{\frac{(1 + \kappa y)}{(1 + \gamma y)(y_m - y)y(1 - y)}} dy, \quad (5)$$

$$I_R(y_b, y_m) = \int_{y_b}^{y_m} \sqrt{\frac{(1 + \kappa y)(1 + \gamma y)(1 - y)}{(y_m - y)y[1 - \nu(1 - y)]}} \times \frac{dy}{1 + \sqrt{1 - \nu(1 - y)}}, \quad (6)$$

$$I_C(y_b, y_m) = \int_{y_b}^{y_m} \sqrt{\frac{(1 + \kappa y)(1 + \gamma y)}{(y_m - y)y(1 - y)}} dy. \quad (7)$$

where $\kappa = (K_3 - K_1)/K_1$.

The balance of torques at the boundary gives the expression for the anchoring coefficient

$$W = \frac{2K_1 I_C}{d \sin 2(\theta - \theta_p)} \sqrt{\frac{(1 + \kappa y_b)(y_m - y_b)}{(1 + \gamma y_b)}}. \quad (8)$$

In the HEF technique, W is determined in voltage region (V_{\min} , V_{\max}) where the integrals in Eqs. (5)–(7) can be simplified. When $V > V_{\min} = 6V_{th}$,² then $1 - y_m < 3 \times 10^{-6}$. This allows replacing y_m with 1 in I_R , while I_C and I_V have the logarithmic singularities $\propto |\ln(1 - y_m)|$. Second, the deviation from the easy axis should be small, allowing for a natural expansion of the integrals in terms of $\sin(\theta - \theta_p)$ and keeping only the linear term of the expression. Limiting deviations to $|\theta - \theta_p| < 0.2$ radians, one gets the upper voltage limit:

$$V < V_{\max} = \frac{0.2}{\pi \cos \theta_p} \sqrt{\frac{\epsilon_{\perp}}{\epsilon_{\parallel}}} \frac{Wd}{K_1} V_{th}.$$

Within (V_{\min} , V_{\max}), the product RCV can be written as a linear function of CV with a coefficient proportional of W^{-1} :

$$\frac{RCV}{R_0} = J_0 - \frac{2K_1}{dW} (1 + \kappa \sin^2 \theta_p) CV, \quad (9)$$

where J_0 is a constant, and R_0 is the retardation under no external field. Also, the capacitance can be written as

$$CV = \frac{\epsilon_0 \epsilon_{\parallel} S}{Qd} (V - \bar{V}), \quad (10)$$

where

$$Q = 1 - \frac{2K_1}{Wd} \frac{\gamma(1 + \kappa y_p)(1 - y_p)}{(1 + \gamma y_p)}, \quad \bar{V} = \alpha \frac{\epsilon_a}{\epsilon_{\parallel}} V_{th},$$

and

$$\alpha = \frac{1}{\pi} \int_{y_p}^1 \sqrt{\frac{(1 + \gamma)(1 + \kappa y)}{y(1 + \gamma y)}} dy.$$

Equation (10) is valid over the same voltage range (V_{\min} , V_{\max}) as Eq. (9). For most liquid crystals with positive $\gamma > 0$ and $\kappa > 0$, the coefficient α is between $2/\pi$ and 1. Substituting Eq. (10) into Eq. (9), we have the final equation to determine W :

$$\frac{R(V - \bar{V})}{R_0} = \tilde{J}_0 - \frac{2K_1}{Wd} (1 + \kappa y_p)(V - \bar{V}), \quad (11)$$

where \tilde{J}_0 is a constant. Note that the condition on V_{\max} requires *a priori* knowledge of W , however, one can show that this condition will be satisfied if the contribution of linear term does not exceed 20% of the constant term in Eq. (9) or Eq. (11).

Experiment: A liquid crystal cell was assembled from substrates coated with a Nissan PI2555 alignment layer. First, indium tin oxide was patterned on the glass substrate to create electrodes. Second, the alignment layer on the glass was prepared by spin coating a 1:4 solution of Nissan polyimide PI2555 in the solvent HD MicroSystems T9039 onto the substrates, baking for 1 h at 275 °C, and mechanical rubbing. Two substrates were assembled into a cell such that the rubbing directions at the plates were antiparallel. The cell gap fixed by Mylar strips was measured to be 27 μm by an interference method. The optical phase retardation of the empty cell was measured to be 0.8° by the Senarmont technique.

The cell was filled with the liquid crystal 4-*n*-pentyl-4'-cyanobiphenyl 5CB (EM Industries). The properties of 5CB at 23 °C are as follows: $K_1 = 6.65 \times 10^{-12}$ N and $K_3 = 8.95 \times 10^{-12}$ N;⁷ $n_e = 1.717$, $n_o = 1.530$, measured in the laboratory. To assure the most accurate implication of the experimental techniques, we measured $\epsilon_{\perp} = 8.0$ and $\epsilon_{\parallel} = 19.5$ before and after the measurement of optical retardation and capacitance. The pretilt angle of the cell was determined to be 3° by the magnetic null method.⁸ All measurements were performed at 23 °C.

To determine W using the HEF technique, the cell capacitance and optical phase retardation must be measured as a function of applied voltage. Before running the experiment, the capacitance of the cell was measured using a Schlumberger SI1260 impedance analyzer. This serves as an experimental check of the bulk properties of the liquid crystal through determination of the threshold voltage, as well as an

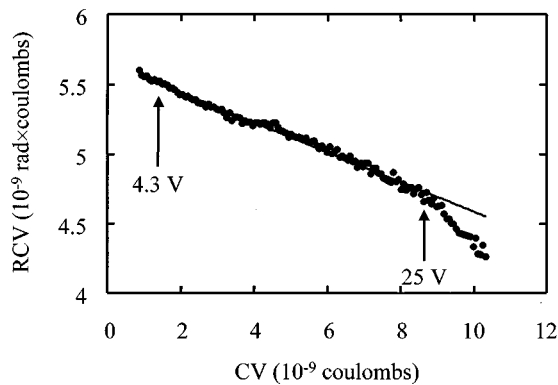


FIG. 2. The dependence of RCV plotted against CV . The solid line represents the best linear fit through the data from 4.3 to 25 V, and yields $W = 2.3 \times 10^{-4} \text{ J/m}^2$.

accurate measure of the capacitance. Leads are then attached to the cell, and it is placed in the experimental setup for the determination of anchoring. The cell is driven by a Stanford Research Systems Model DS345 function generator amplified by a Krohn-Hite Model 7600 wide band amplifier. The 60 kHz sinusoidal potential is routed into a cell and a 30 k Ω resistor in series, and the potential drop across the resistor is measured. The voltage drop across the resistor is considered when determining the voltage across the cell. Since the resistance of the cells used was larger than 3 M Ω , and, thus, gave negligible contributions to the total impedance, the capacitance of the cell can be determined. Since the leads to the cell also add a capacitance, the results of this experiment are compared with the capacitance measured with the Schlumberger SI1260 impedance analyzer, with the appropriate constant subtracted off of the former results. This gives C with an uncertainty of 1 pF.

The optical phase retardation of the liquid crystal cell is determined using the Senarmont technique with a low power He-Ne laser. Linearly polarized light at 45 $^\circ$ with the rubbing direction impinges on the sample. The light emerging from the sample is elliptically polarized and transformed back into linearly polarized light by a quarter wave plate. The angle of the linearly polarized light was determined by rotating the analyzer to determine the point of extinction. The absolute uncertainty in the measured phase retardation is 0.5 $^\circ$.

Figure 2 shows the plot of RCV against CV for the cell. The contribution due to the retardation from the cell's substrates is subtracted off. By performing a linear fit from $V_{\min} = 6V_{th} = 4.3 \text{ V}$ to $V_{\max} = 25 \text{ V}$, Eq. (9) yields $W = 2.3 \pm 0.3 \times 10^{-4} \text{ J/m}^2$. The uncertainty quoted here reflects only uncertainties in the measured parameters. The possibility of systematic errors affecting the "high-electric-field" technique will be discussed in a future work.⁹

Figure 3 shows the plot of $R(V - \bar{V})$ and CV vs $(V - \bar{V})$ for the same cell. Note that the dependence of CV on $(V - \bar{V})$ is linear with a zero intercept, in agreement with Eq.

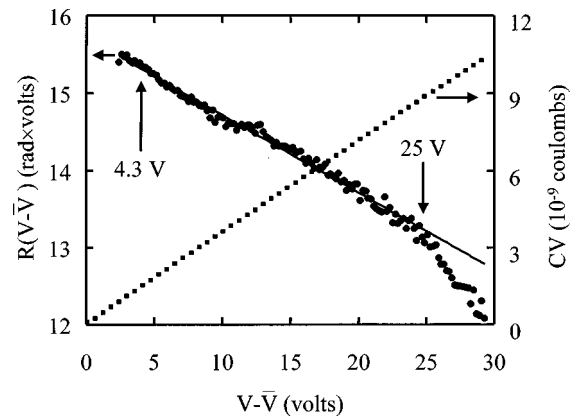


FIG. 3. The dependence of $R(V - \bar{V})$ (circles; left-hand side scale) and CV (small squares; right-hand side scale) plotted against $(V - \bar{V})$. The solid line represents the best linear fit through the data from 4.3 to 25 V, and yields $W = 2.5 \times 10^{-4} \text{ J/m}^2$.

(10). For 5CB in a cell with 3 $^\circ$ pretilt, $\alpha = 0.828$ and $\bar{V} = 0.39 \text{ V}$. With this result and fitting the experimental data from $V_{\min} = 4.3 \text{ V}$ to $V_{\max} = 25 \text{ V}$, Eq. (11) yields $W = 2.5 \pm 0.3 \times 10^{-4} \text{ J/m}^2$. The accuracy of \bar{V} has a small effect on the resultant W .⁹

We demonstrated a way to significantly simplify the determination of W by the high-electric-field technique. One should bear in mind, however, that both RV and the standard HEF technique are equally vulnerable to in-plane inhomogeneities of tested cells. Note that the theoretical models in both cases are based on a one-dimensional image of director distortions. In real cells, the in-plane inhomogeneities (e.g., variations of the easy axis and the associated anchoring potential) lead to significant deviations from the ideal theoretical response of the cell. The analysis of these deviations will be published elsewhere.⁹

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