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Determination of the surface anchoring potential of a nematic in contact with a substrate

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We have developed a method for determining the surface anchoring potential for nematics in contact with a substrate that provides director alignment. Our main result is that the surface torque and hence the anchoring potential may be determined from either dielectric or optical phase response of a nematic undergoing a Freedericksz transition. The method is based on the Frank–Oseen continuum theory, and makes no assumptions about the functional form of the potential. We have measured the surface anchoring potential of two types of substrate in contact with the nematic liquid crystal 4-*n*-pentyl-4′-cyanobiphenyl. The surfaces were ITO-coated float glass, coated either with obliquely evaporated SiO or a buffed polymer film. Comparison of the results obtained from capacitance and optical measurements provides an estimate of the goodness of the method.

1. Introduction

In this paper we propose a method for determining the surface anchoring potential of substrates in contact with a nematic liquid crystal. We consider a nematic between plane-parallel boundaries undergoing an electric-field-induced splay Freedericksz transition. If the material parameters of the nematic are known then the anchoring potential of the substrate may be determined as a function of the director orientation from the capacitance-versus-voltage data. The method involves the calculation of the director angle at the substrate surface from experimental data using an analytic expression for the deformation in the cell, and then calculating the corresponding surface torque. The surface torque as a function of the director angle may be integrated to yield the surface anchoring potential. An analogous procedure may be carried out using the optical phase shift versus voltage data. This can serve as an independent check on the results.

We have applied this method to determine the surface anchoring potential of both tangentially evaporated SiO and a buffed polymer film on glass plates in contact with the liquid crystal 4-*n*-pentyl-4′-cyanobiphenyl (5CB) from both capacitance and optical phase-shift data. The anchoring strength is the curvature of the surface potential at zero deformation angle, and we found that the anchoring strength of the buffed polymer film is comparable to that of the SiO layer.

2. Theory

The surface anchoring potential is a measure of the free-energy cost of changing the angle that the director makes with the plane of the surface. The subject was first discussed by Rapini and Papoular [1]; a comprehensive review is given in [2].

The geometry that we consider consists of two infinite conducting planes given by $z = 0$ and $z = d$. The boundary conditions are such that the director is in the x

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direction at these boundaries in the undistorted configuration. We assume that the director $\hat{\mathbf{n}}$ always lies in the xz plane; its direction is then specified by the angle ϕ where $\cos\phi = \hat{\mathbf{n}} \cdot \hat{\mathbf{x}}$. In this geometry the free energy of deformation per unit area is [3]

$$F_d = \frac{1}{2}\int_0^d (K_1 \cos^2\phi + K_3 \sin^2\phi)\left(\frac{\partial\phi}{\partial z}\right)^2 dz, \tag{1}$$

where K_1 and K_3 are respectively the splay and bend elastic constants.

In order to derive the equation of state, it is convenient to consider the thermodynamic potential

$$F = F_d + \int_0^d \tfrac{1}{2}\mathbf{D}\cdot\mathbf{E}\, dz. \tag{2}$$

The z component of the electric field is related to the displacement by $E_z = \varepsilon_0\varepsilon_{33}D$, where

$$\varepsilon_{33} = \varepsilon_\parallel \sin^2\phi + \varepsilon_\perp \cos^2\phi. \tag{3}$$

Thus the thermodynamic potential to be minimized is

$$F = \frac{1}{2}\int_0^d \left[(K_1 \cos^2\phi + K_3 \sin^2\phi)\left(\frac{\partial\phi}{\partial z}\right)^2 + \frac{D^2}{\varepsilon_0(\varepsilon_\parallel \sin^2\phi + \varepsilon_\perp \cos^2\phi)}\right] dz. \tag{4}$$

This differs from the potential used by Deuling [4], but leads more directly to the same Euler–Lagrange equation satisfied by $\phi(z)$. This may be integrated once, and the constant of integration is determined from the condition that $\partial\phi/\partial z = 0$ at $z = \frac{1}{2}d$. Here $\phi = \phi_m$, and a second integration gives

$$\frac{D}{D_0} = \frac{2}{\pi}(1 + \gamma \sin^2\phi_m)^{1/2}\int_{\phi_1}^{\phi_m}\left[\frac{(1 + \kappa \sin^2\phi)(1 + \gamma \sin^2\phi)}{\sin^2\phi_m - \sin^2\phi}\right]^{1/2} d\phi, \tag{5}$$

where $\kappa = K_3/K_1 - 1$ is the anisotropy of the elastic constants, and $\gamma = \varepsilon_\parallel/\varepsilon_\perp - 1$ is a reduced dielectric anisotropy.

$$D_0 = \frac{\pi}{d}\left(\frac{K_1\varepsilon_0\varepsilon_\perp}{\gamma}\right)^{1/2}$$

and ϕ_1 is the second constant of integration and also the director angle at the substrate surface. The cell voltage is given by

$$V = \int_0^d \varepsilon_0\varepsilon_{33} D\, dz;$$

changing the variable of integration results in

$$\frac{V}{V_0} = \frac{2}{\pi}(1 + \gamma \sin^2\phi_m)^{1/2}\int_{\phi_1}^{\phi_m}\left[\frac{1 + \kappa \sin^2\phi}{(\sin^2\phi_m - \sin^2\phi_1)(1 + \gamma \sin^2\phi)}\right]^{1/2} d\phi, \tag{6}$$

where

$$V_0 = \pi\left(\frac{K_1}{\varepsilon_0\varepsilon_\perp\gamma}\right)^{1/2}.$$

In the case of finite anchoring, the Freedericksz transition occurs at a voltage $V_{th} < V_0$. In our geometry, however, the relative difference between these quantities [5] is expected to be $\lesssim 10^{-3}$; we therefore take $V_0 = V_{th}$.

The deformation in the cell, $\phi(z)$, is determined completely by either V and D or equivalently by ϕ_m and ϕ_1. Furthermore, since the displacement is simply the surface charge density, it is given by

$$D = CV/A, \tag{7}$$

where A is the area of the plates and C is the capacitance. For given values of C and V, equations (5) and (6) may, in principle, be solved for ϕ_m and ϕ_1.

Torque balance at the substrate surface requires that

$$\frac{\partial W}{\partial \phi_1} = K_1(1 + \kappa \sin^2 \phi_1) \left.\frac{\partial \phi}{\partial z}\right|_{z=0}, \tag{8}$$

where $W(\phi_1)$ is the surface anchoring potential; $\partial\phi/\partial z$ is known from the first integral of the Euler–Lagrange equation. Thus if equations (5) and (6) can be inverted to yield ϕ_1 and ϕ_m then the right-hand side of the torque-balance equation can be evaluated and $\partial W/\partial\phi_1$ can be integrated to yield the surface anchoring potential.

We now describe our procedure for inverting equations (5) and (6). The integrands in these equations are singular at the upper limit and hence these integrals are not amenable to numerical integration. We therefore make the change of variables used by Deuling [4]:

$$\sin \phi = \sin \psi \sin \phi_m$$

and

$$\eta = \sin^2 \phi_m.$$

This results in

$$cv = \frac{2}{\pi}(1+\gamma\eta)^{1/2} \int_{\psi_1}^{\pi/2} \left[\frac{(1 + \kappa\eta \sin^2 \psi)(1 + \gamma\eta \sin^2 \psi)}{1 - \eta \sin^2 \psi}\right]^{1/2} d\psi, \tag{9}$$

where $c = C/C_0$ and $v = V/V_{th}$, C_0 is the zero-field capacitance and

$$\psi_1 = \arcsin \sin \phi_1/\sin \phi_m.$$

Similarly, equation (6) can be rewritten as

$$v = \frac{2}{\pi}(1 + \gamma\eta)^{1/2} \int_{\psi_1}^{\pi/2} \left[\frac{1 + \kappa\eta \sin^2 \psi}{(1 - \eta \sin^2 \psi)(1 + \gamma\eta \sin^2 \psi)}\right]^{1/2} d\psi. \tag{10}$$

The problem is then reduced to solving for η and ψ_1. The integrands are rapidly varying functions of ψ for $\eta \approx 1$, and to enable numerical integration we rewrite the integrals in the form [6]

$$\int_{\psi_1}^{\pi/2} \frac{f(\psi)\, d\psi}{(1 - \eta \sin^2 \psi)^{1/2}} = \int_{\psi_1}^{\pi/2} \frac{[f(\psi) - f(\tfrac{1}{2}\pi)]\, d\psi}{(1 - \eta \sin^2 \psi)^{1/2}} + f\left(\frac{\pi}{2}\right) \int_{\psi_1}^{\pi/2} \frac{d\psi}{(1 - \eta \sin^2 \psi)^{1/2}}. \tag{11}$$

The first term on the right-hand side is well behaved and can be evaluated by an adaptive Simpson's-method algorithm. The second can be expressed as a sum of complete and incomplete elliptic integrals. We further note that, while, η is good parameter for describing the amount of distortion in the cell, when the cell voltage

becomes appreciably greater than threshold, $\eta - 1$ becomes so small as to result in computer underflow error. We therefore make the further substitution [6] $\eta = 1 - \exp(-\alpha)$. These substitutions make the evaluation of equations (9) and (10) numerically tractable. The procedure used to invert these equations was a two-dimensional fixed-point iteration. If the equations are written as

$$cv = f_1(\alpha, \psi_1), \quad v = f_2(\alpha, \psi_1) \tag{12}$$

then the iteration scheme is

$$\begin{bmatrix} \alpha \\ \psi_1 \end{bmatrix}_{i+1} = \begin{bmatrix} \alpha \\ \psi_1 \end{bmatrix}_i + \begin{bmatrix} \partial f_1/\partial\alpha & \partial f_1/\partial\psi_1 \\ \partial f_2/\partial\alpha & \partial f_2/\partial\psi_1 \end{bmatrix}^{-1} \begin{bmatrix} cv - f_1 \\ v - f_2 \end{bmatrix}\Bigg|_{\substack{\alpha=\alpha_i \\ \psi_1=\psi_{1i}}}. \tag{13}$$

The derivatives appearing in this expression were evaluated using the same techniques as were used for the functions f_1 and f_2. Initial guesses are made for α and ψ_1, and α_i and ψ_{1i} are the ith improvements on the guesses. Iteration proceeds until the convergence criteria are met; these criteria are that the difference between successively iterated values be less than an error limit, typically 10^{-7}. Rapid convergence was obtained everywhere except in the domain $\alpha = 19{\cdot}5 \pm 0{\cdot}3$. The reasons for this lack of convergence are not well understood. The program was tested by using computer-generated data.

In addition to capacitance, the optical response of the cell may be considered. We define δ as the phase difference between ordinary and extraordinary rays, and Θ as the reduced phase; $\Theta = 1 - \delta/\delta_0$, where δ_0 is the phase difference for the cell at zero voltage. The reduced phase is given by

$$\left(1 - \frac{n_e}{\Delta n}\Theta\right) cv = \frac{2}{\pi}(1 + \gamma\eta)^{1/2} \int_{\psi_1}^{\pi/2} \left[\frac{(1 + \kappa\eta \sin^2\psi)(1 + \gamma\eta \sin^2\psi)}{(1 - \eta \sin^2\psi)(1 + \nu\eta \sin^2\psi)}\right]^{1/2} d\psi, \tag{14}$$

where $\nu = n_e^2 n_0^2 - 1$ and Δn is the birefringence. This equation can be used in place of equation (9) to solve for α and ψ_1; these values may be used to verify the results of the first method.

3. Experimental

Indium tin oxide coated glass plates were prepared using two different surface-alignment techniques: SiO deposited from the vapour at an oblique angle and a polymer film deposited on the substrate from solution and then buffed. After preparation, the plates were separated by 38 μm mylar spacers and filled by capillary action with the liquid crystal 5CB (obtained from BDH Chemicals) in the isotropic phase. The samples were examined using a polarizing microscope; both the surface treatments resulted in uniform homogeneous alignment. The thickness of the nematic layer was determined by optical interference methods [7]. The cells prepared were placed in a thermostatted housing with temperature control of better than ± 1 mK. The cell voltage was applied through the ratio transformer of a GenRad 1615A capacitance bridge. The voltage was monitored with a $4\frac{1}{2}$ digit DMM and controlled by a microcomputer. The capacitance bridge enabled measurement of the capacitance with accuracy better than $\pm 0{\cdot}005$ per cent. The voltage response was measured from 0 to 100 V r.m.s. An example of a C–V response curve is shown in figure 1; the region in

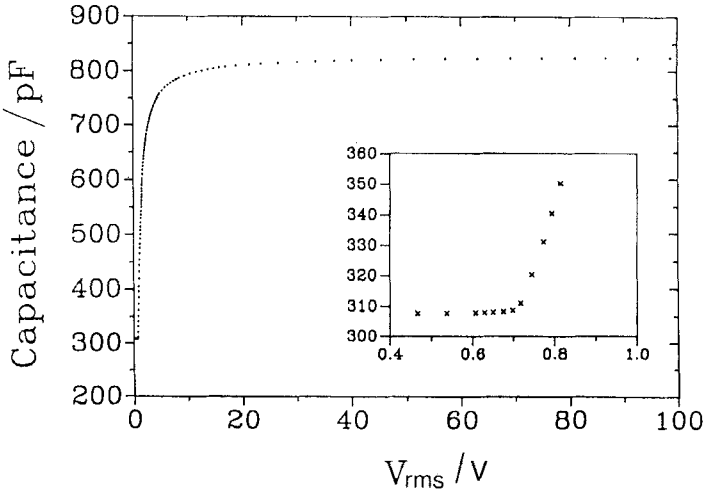

Figure 1. Example of capacitance-versus-voltage data. The region of the threshold is expanded in the inset.

the vicinity of the threshold is shown in the inset. Phase-retardation data was obtained using a method similar to that described by van Sprang [8].

4. Analysis of data

In order to utilize the method outlined here, it is necessary to know the values of material constants. Both elastic constants (K_1 and K_3), the principal values of the dielectric tensor, and the birefringence could be determined from our experimental data. The values of the average refractive index were taken from [9]. Using these values, equations (9) and (10) were inverted as outlined previously to yield ϕ_1 and ϕ_m as functions of the cell voltage. Figure 2 shows the results of this fit for ϕ_1

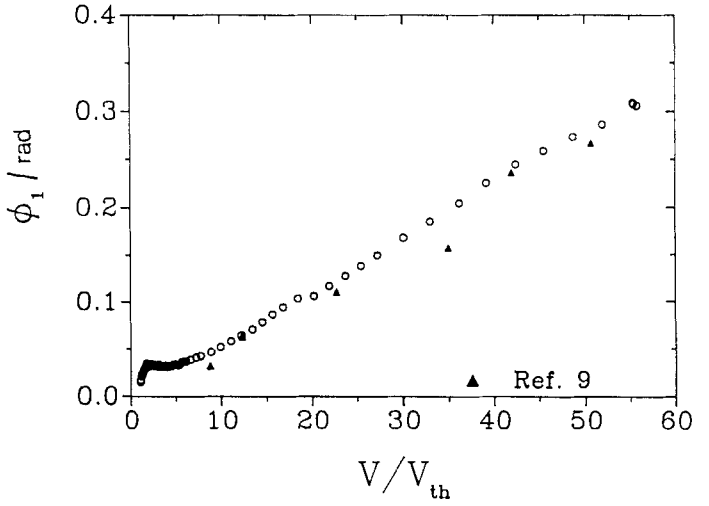

Figure 2. Director angle at the substrate surface plotted against the reduced cell voltage for obliquely evaporated SiO surface treatment. The results of [9] are included for comparison (▲).

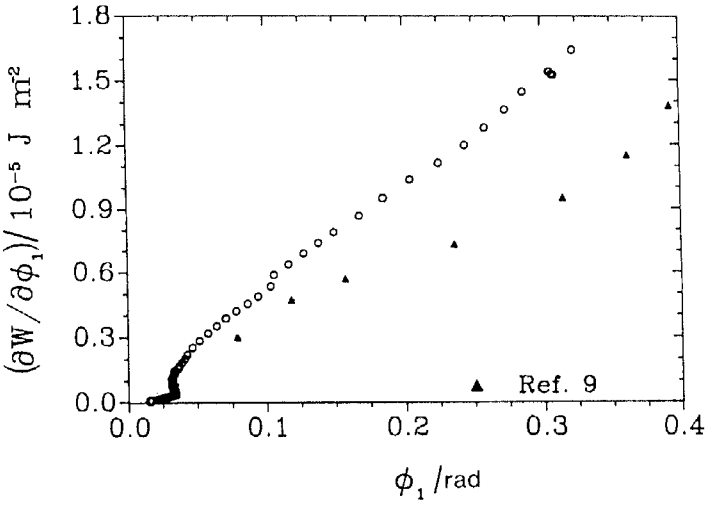

Figure 3. Derivative of the surface anchoring potential as a function of director angle at the surface for obliquely evaporated SiO surface treatment. The results of [9] are included for comparison (▲).

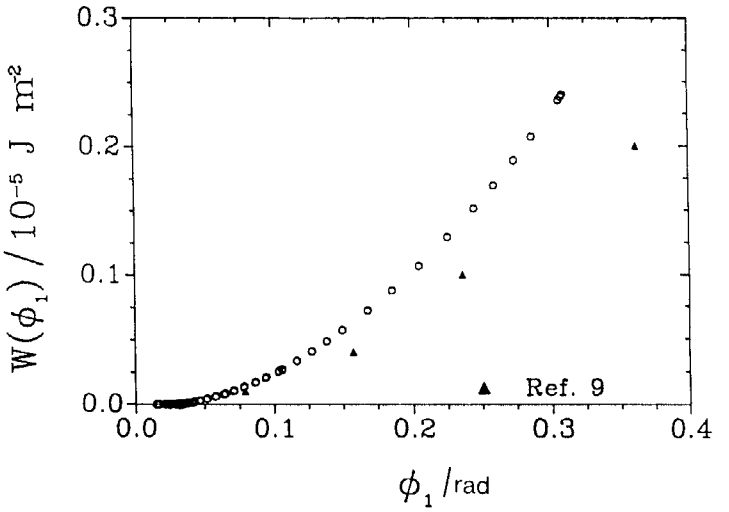

Figure 4. Surface anchoring potential for obliquely evaporated SiO surface treatment as a function of the director angle at the surface. The results of [9] are included for comparison (▲).

for SiO-treated glass. The graph includes the results obtained by Yokoyama and van Sprang [9] for the same surface treatment; their results were obtained using a different approach, which requires both capacitance and optical phase data. The value of ϕ_1 can be used in the torque-balance equation (i.e. equation (8)) to obtain the derivative of the anchoring potential $\partial W/\partial\phi_1$. This is shown in figure 3, again for SiO-treated plates, together with the results from [9]. Finally, this curve can be integrated to yield $W(\phi_1)$, the surface anchoring potential; this is shown in figure 4. Corresponding results for the buffed polymer surface are shown in figures 5–7.

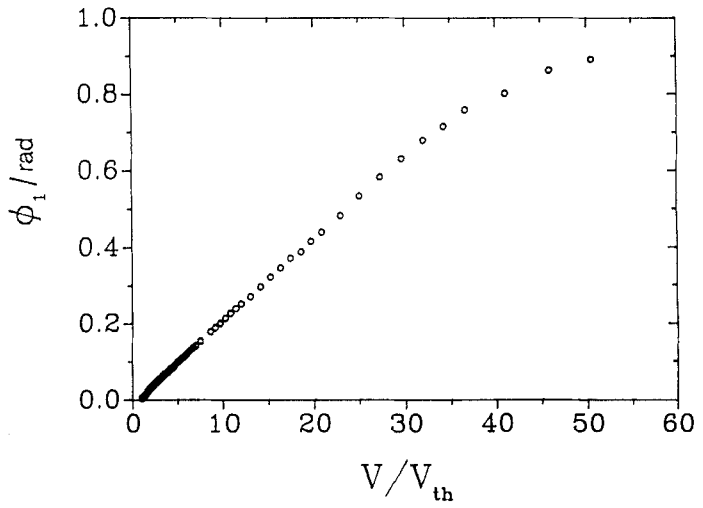

Figure 5. Director angle at the substrate surface plotted against reduced cell voltage for buffed-polymer-film surface treatment.

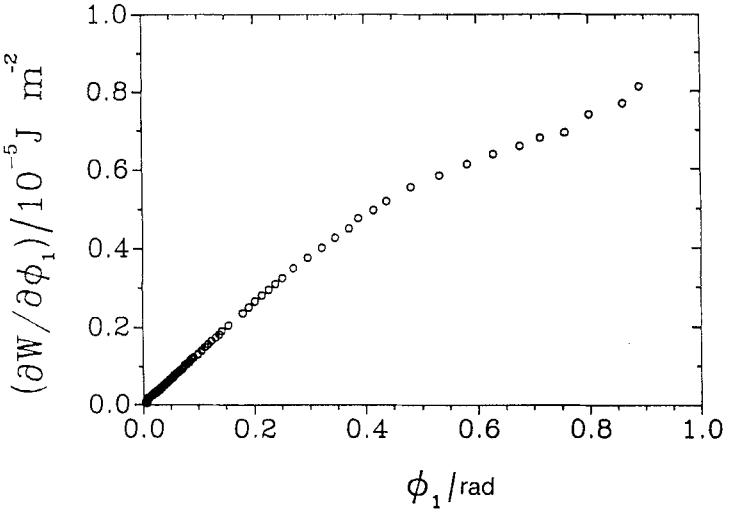

Figure 6. Derivative of the surface anchoring potential as a function of the director angle at the surface for buffed-polymer-film surface treatment.

5. Discussion

The results of this numerical analysis were found to be sensitive to the values of the material constants used, particularly to the value of γ. While these values were obtained directly from our experimental data, the associated uncertainty (typically $\pm 0{\cdot}5$ per cent for γ) was large enough to affect the results significantly. The resulting uncertainty in ϕ_1 and subsequently calculated quantities was greatest for large cell voltages. The sensitivity of $\partial W/\partial\phi_1$ is shown in figure 8. We therefore believe that our method is most useful in the region of small voltages (and tilt angles). When this method was applied to the optical phase data, the results showed considerable scatter. The reason for this is not fully understood. As a consequence, we have found optical

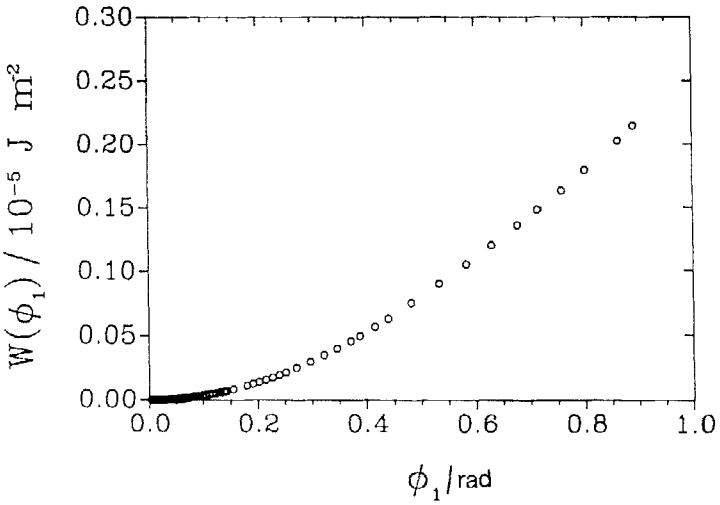

Figure 7. Surface anchoring potential for buffed-polymer-film surface treatment as a function of the director angle at the surface.

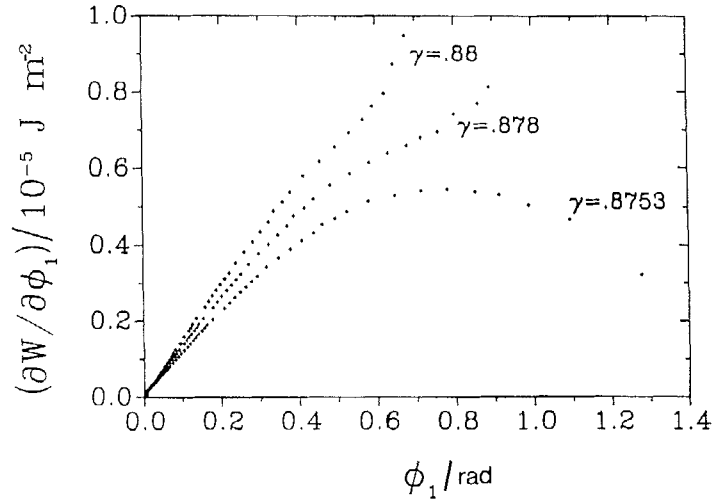

Figure 8. Derivative of the surface anchoring potential as a function of director angle at the surface. The different curves correspond to different values of γ used in fitting the data with our method.

phase measurements to be less useful than capacitance data for the purpose of this analysis.

We believe that the method described here is a useful way of determining the surface anchoring potential with no *a priori* assumptions about its functional form. The method is particularly useful in the region of smaller tilt angles, and is expected to yield reliable results for all angles if the material constants are known with sufficient accuracy.

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