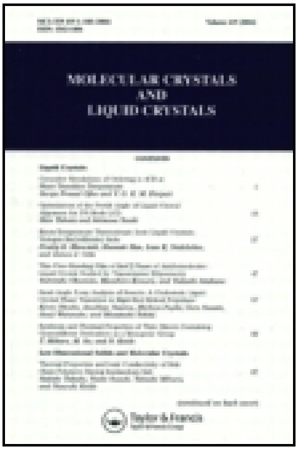

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Influence of the Microtopography of the SiO Covered by PVA Layers on the Tilt Angle of Liquid Crystals

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Version of record first published: 23 Sep 2006.

To cite this article: R. Moldovan , S. Frunzå , T. Beica & G. Barbero (1994): Influence of the Microtopography of the SiO Covered by PVA Layers on the Tilt Angle of Liquid Crystals, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 257:1, 125-130

To link to this article: http://dx.doi.org/10.1080/10587259408033769

Mol. Cryst. Liq. Cryst., 1994, Vol. 257, pp. 125–130
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Influence of the Microtopography of the SiO Covered by PVA Layers on the Tilt Angle of Liquid Crystals

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An evaluation of the tilt angle variation observed recently when unrubbed polyvinylic alcohol is deposited on obliquely evaporated SiO layers is presented. The method of calculation supposes that the variation of the tilt angle is due to the modification of the initial topography of SiO during the coverage process with the polymeric film. The Laplace equation was obtained by minimizing the elastic energy of the system in the uniconstant approximation and was analytically solved. The found variation of the tilt angle is in good agreement with the experimentally observed one.

INTRODUCTION

It is well known that silicon monoxide films evaporated at an incidence angle greater than 80° to the glass substrates exibit an aligning influence on the molecules of liquid crystals. The molecular director is tilted out of the plane of the glass and points towards the direction of evaporation.

Using the elastic-energy model firstly proposed by Guyon *et al.*[1] and a measured columnar structure of these films and assuming that the director is locally parallel to the surface everywhere, Goodman *et al.*[2] have predicted that the molecular director in the bulk of the fluid should be slightly greater than the angle of inclination of the columns with the substrate. In this form the model could not explain some experimental observations made by several authors as the dependence of the tilt angle on the liquid crystal nature and on the temperature. These dependences were however evidenced by using a phenomenological treatment of the surface interaction energy of the liquid crystal with the solid substrate for the determination of the local direction of the director at the solid surface[3,4] and taking into account the influence of the topography.[5]

Another alignment method consists in using rubbed thin polymer films. Although the mechanism of alignment was firstly considered to be essentially topographic, recent studies show that the liquid crystal alignment is due to the *unidirectional* oriented crystalline structure obtained by the rubbing process. The alignment of liquid crystal molecules is imposed by the orientation of polymeric chains on the surface of the rubbed films,[6,7] as well as on stretched polymer films[8] or on Langmuir-Blodgett deposited films.[9]

The mechanism of uniform alignment of liquid crystal molecules is still a matter of study.

Recently[10] a new method of producing tilted molecular orientation in nematic liquid crystal cells using unrubbed polyvinylic alcohol (PVA) films was reported. This method consists in the covering of an obliquely evaporated SiO layer by a thin film of PVA and permits to obtain a continuous variation of the tilt angle from 30° (uncovered SiO layers) to 7°, as function of the concentration of the used PVA solutions. In this paper we present an evaluation of the tilt angle variation by using a calculation method proposed by some of us.[11] We supposed that the variation of the tilt angle is due to the modification of the initial topography of SiO by shortening of the columns of the topograpgy, the PVA laying preferably in the hollows.

THEORETICAL APPROACH

The profile of the surface topography of the SiO deposited films in the incidence plane is supposed to consist of a periodic succession of columns inclined towards the substrate and having a face perpendicularly oriented to the SiO deposition direction (see the part A of Figure 1). The manner in which the PVA covering of the SiO microtopography takes place is difficult to be specified. For sake of simplicity and in order to outline the importance of the topography in the molecular alignment mechanism, we considered that the microtopography modification is mainly caused by the shortening of the column lengths, the other parameters remaining unchanged. We assumed that the director is locally parallel to the surface everywhere because it is known that the director possesses random parallel orientation on unrubbed PVA films, and, in addition that it can lie only in the incidence plane of SiO deposition.

In the following, the microtopography obtained by SiO deposition is considered as equivalent with a planar surface characterized by three easy axes, as shown in the part B of Figure 1.

We denoted by $\theta_0(x)$ the easy axis on the equivalent planar surface.

Therefore:

$$\theta_0(x) = \begin{cases} \alpha & \text{for } 0 \leq x < a \\ \beta & \text{for } a \leq x < b \\ \gamma & \text{for } b \leq x < \lambda \end{cases} \tag{1}$$

The cell considered in the calculation consists of two such boundary surfaces mounted in a symmetrical way as shown in Figure 2. The total elastic free energy was

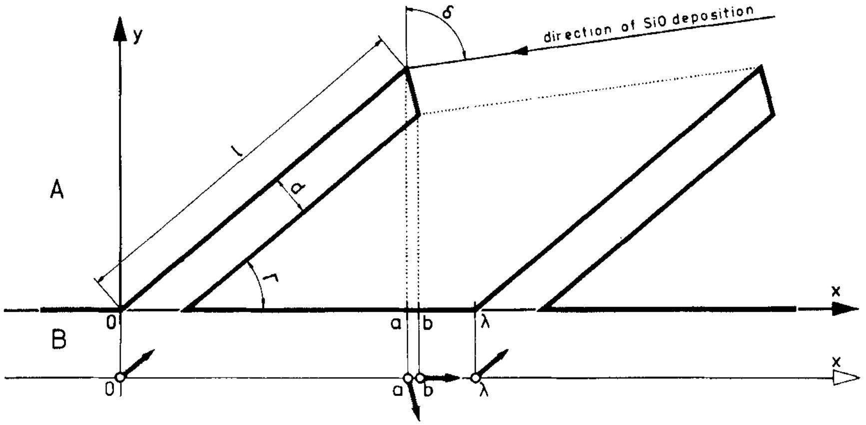

FIGURE 1 The equivalence of a columnar microtopography having local easy direction parallel to the solid surface (A) with a planar surface (B) with three inclined easy directions.

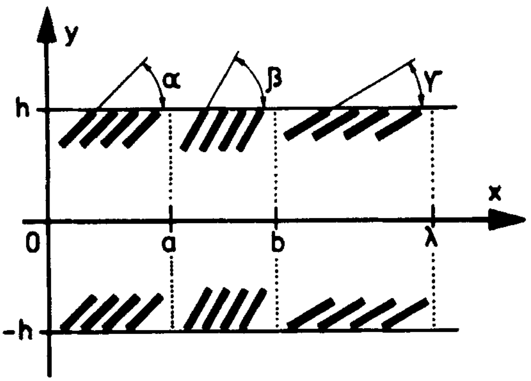

FIGURE 2 The geometry of a symmetrical assembled liquid crystal cell.

expressed for one period of a half of the nematic sample thickness, in the uniconstant approximation:

$$F = \frac{1}{2}k\int_{-h}^{0}\int_{0}^{\lambda}(\nabla\theta)^2\,dx\,dy + \frac{1}{2}W\int_{0}^{\lambda}[\theta(x,-h)-\theta_0(x)]^2\,dx \qquad (2)$$

In Equation (2) the first term represents the energy due to the bulk distortion and the second, the surface energy, W beeing the anchoring energy supposed to have the same value for any x. The equilibrium configuration is obtained by minimizing Equation (2), that leads to:

$$\frac{\delta^2\theta}{\delta x^2} + \frac{\delta^2\theta}{\delta y^2} = 0 \qquad (3)$$

with the boundary condition at $y = -h$:

$$-\left.\frac{\delta\theta}{\delta y}\right|_{y=-h} + \frac{1}{L}[\theta(x, -h) - \theta_0(x)] = 0 \tag{4}$$

where $L = k/W$.

We observe that the total free energy is minimized by an armonic function which has to satisfy the boundary condition (4). Following the method from Reference 11 we find the solution of Equation (3) by expanding $\theta(x, y)$ in a Fourier series and taking into account that it has to be an even function with respect to the middle of the sample thickness. Then we suppose that:

$$\theta(x, y) = \frac{D_0}{2} + \sum_{n=1}^{\infty} [D_n \cos(nqx) + E_n \sin(nqx)]ch(nqy) \tag{5}$$

where $q = 2\pi/\lambda$ and ch is the hyperbolic cosinus. Replacing Equation (5) in condition (4) we obtain the expansion coefficients:

$$\begin{aligned}
\frac{D_0}{2} &= \frac{\alpha a + \beta(b-a) + \gamma(\lambda - b)}{\lambda}\\
D_n &= \frac{2}{\lambda}\frac{(\alpha-\beta)\sin(nqa) + (\beta-\gamma)\sin(nqb)}{nq[nqLsh(nqh) + ch(nqh)]}\\
E_n &= \frac{2}{\lambda}\frac{(\alpha-\beta)[1-\cos(nqa)] + (\beta-\gamma)[1-\cos(nqb)]}{nq[nqLsh(nqh) + ch(nqh)]}
\end{aligned} \tag{6}$$

The equivalent direction, θ_E, of a uniform surface that would replace the considered periodically variable one, was chosen as the value for what the relation:

$$\theta_E^2 = \langle\theta^2\rangle \tag{7}$$

is satisfied, where

$$\langle\theta^2\rangle = \frac{1}{2h\lambda}\int_0^{\lambda}\int_{-h}^{h} \theta^2(x, y)\,dx\,dy. \tag{8}$$

Performing the calculations we obtain:

$$\begin{aligned}
\theta_{E^2} = {} & \left[\frac{\alpha a + \beta(b-a) + \gamma(\lambda-b)}{\lambda}\right]^2\\
& + \frac{4}{h}\frac{(\alpha-\beta)(\alpha-\gamma)}{\lambda^2}\sum_{n=1}^{\infty}\frac{\sin^2(nqa/2)}{(nq)^3(1+nqL)^2}\\
& + \frac{4}{h}\frac{(\alpha-\gamma)(\beta-\gamma)}{\lambda^2}\sum_{n=1}^{\infty}\frac{\sin^2(nqb/2)}{(nq)^3(1+nqL)^2}\\
& + \frac{2}{h}\frac{(\alpha-\beta)(\beta-\gamma)}{\lambda^2}\sum_{n=1}^{\infty}\frac{\sin^2[nq(a-b)/2]}{(nq)^3(1+nqL)^2}
\end{aligned} \tag{9}$$

TABLE I

The Equivalent Easy Direction, θ_E, in Function of the Column Length, l

l (Å)	θ_E (degree)
1000	31
500	15
250	7

where we took into account that $qh = 2\pi h/\lambda \gg 1$ so that:

$$\frac{sh(2nqh) + 2nqh}{[nqLsh(nqh) + ch(nqh)]^2} \approx \frac{2}{(1 + nqL)^2} \tag{10}$$

All the series entering in Equation (9) converge rapidly consequently we can keep only their first terms which are proportional to λ^3 and therefore all the corresponding terms in Equation (9) are proportional to λ/h. As $\lambda/h \ll 1$, all the terms that contain series are very small and

$$\theta_E \approx \frac{\alpha a + \beta(b - a) + \gamma(\lambda - b)}{\lambda} \tag{11}$$

So θ_E is given by the weighted mean of the angles α, β, γ. Therefore a straightforward generalisation of the result given in References 11 is obtained.

The physical parameters of the SiO film were estimated using Goodman's data[2] for a layer thickness measured at normal incidence of 1000 Å (corrected at 120 Å for the geometrical conditions of deposition thickness). Using the notation from Figure 1 (δ—the incidence angle of the SiO deposition, l and d—the length and respectively the width of columns and Γ their inclination, λ—the columnar structure period) these parameters were the following: $\delta = 83°$, $\Gamma = 40°$, $\lambda = 950$ Å, $l = 1000$ Å, $d = 110$ Å. The parameter d was estimated from mass conservation. Under our experimental conditions we observed from Figure 1 that:

$$\alpha = \Gamma,\ \beta = -\delta,\ \gamma = 0,\ a = l \cos\Gamma,\ b - a = d \cos\delta/\sin(\delta + \Gamma)$$

The results for θ_E when l decreases, which corresponds to thicker PVA deposited layers obtained from solutions with increased concentrations, are given in Table 1. The calculated values for θ_E describe well the experimental trend.[10]

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