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The Homogeneous Alignment of Liquid Crystal Layers†‡

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Abstract—The usual way to align a liquid crystal layer homogeneously is rubbing the substrate, whereby micro-grooves are produced. We investigated the orienting influence of micro-grooves of variable density using different substrate materials and different liquid crystals. Some theoretical considerations concerning the aligning effect on liquid crystals of surface deformations are presented.

1. Introduction

The reason for the alignment of a liquid crystal parallel or perpendicular to the supporting walls obviously must be sought in the special type of interaction between liquid crystal (LC) molecules and substrate material. It may be assumed that, in general, a polar interaction will tend to align LC molecules with polar end groups perpendicular to the substrate, and that van-der-Waals interactions will lead to a parallel orientation. These non-polar interactions in general do not result in a uniform alignment, however.

In many technical applications the uniform alignment of nematic liquid crystal layers parallel to the supporting walls ("homogeneous alignment") is of great importance. Chatelain[1] found some 30 years ago that uniformity can be achieved by rubbing the supporting glass plates. New interesting studies on this topic were done by Berreman.[2]

We want to present at first some new experimental details of the Chatelain method and then we treat some underlying theoretical aspects.

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2. Experiments

We found that a very uniform parallel alignment is achieved by use of a polishing tissue impregnated with diamond-paste with a grain size of about 0.25 μm. This simple method yields reproducible results. It is remarkable that the aligning effect of rubbing is essentially independent of the support material, provided that the LC orients parallel to that material.

We got homogeneous alignment by rubbing of glass, lucite, photoresist, MgF_2, SnO_2, In_2O_3, Nesatron and metals such as nickel, aluminum or gold.

We proved by electron-microscopy that the various rubbing methods lead to micro-grooves on the surface (Fig. 1). The density and depth of the micro-grooves depend on the hardness and the

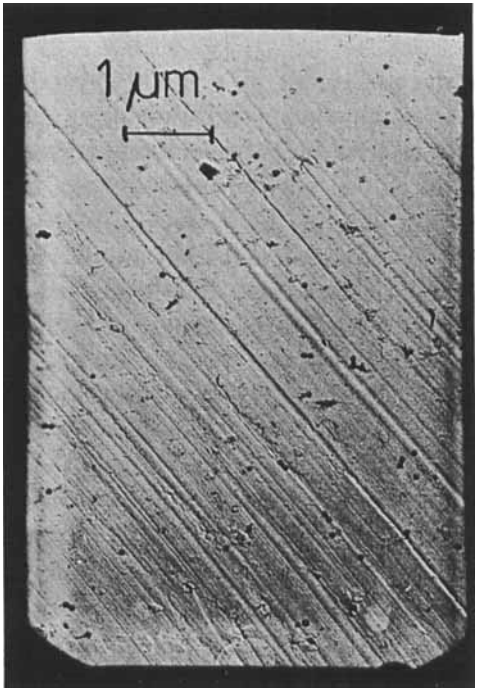

Figure 1. Electron micrograph of a platinum shadowed carbon replica of a tin oxide film rubbed with 1 μm diamond-paste on a DP-cloth.

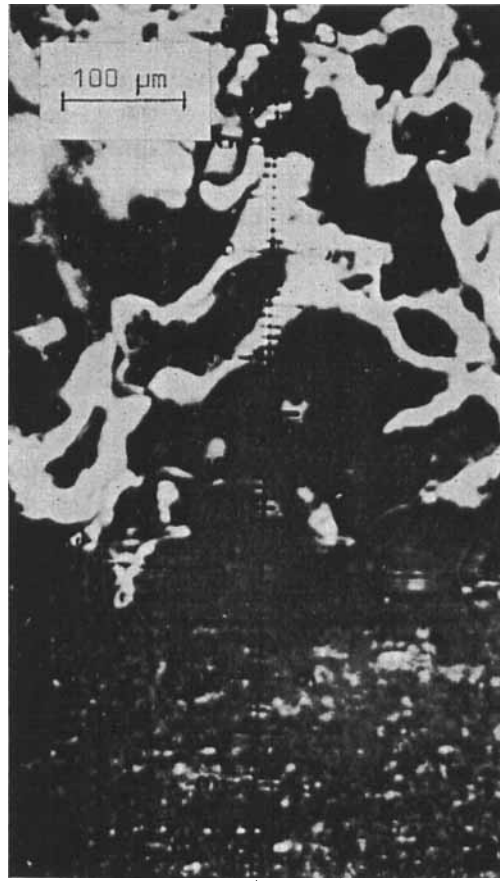

Figure 2. Micrograph of a LC layer between crossed polarizers. The supporting glass plates were partly scratched. Width of scratches: 1 μm; spacing of scratches: 10 μm.

grain size of the abrasive used and upon the hardness of the support material. Microscopic examination showed that the quality of the homogeneous alignment is the better the higher the micro-groove density is. High micro-groove density can be retained especially if the support plate is coated with a soft film, for instance photoresist (AZ 1350 H from Shipley) or a magnesium fluoride film of 0.1 μm thickness and rubbed with a polishing tissue.

To get information about the minimum groove density sufficient

for homogeneous orientation we generated a grating-like structure on different support plates by scratching with a diamond pencil. The distance between the grooves was varied from 2 to 300 μm. It was found that a homogeneous alignment of the nematics MBBA and N5 is achieved, if at a groove width of 1 μm the groove spacing is not larger than 10 μm.

From the micrograph shown in Fig. 2 which was taken with crossed polarizers, it can be seen that in fact the grooves are respon-

Figure 3. Micrograph of a LC layer between crossed polarizers. The supporting glass plates were partly scratched. Width of scratches: 1 μm; spacing of scratches: 25 μm.

sible for the homogeneous alignment of a liquid crystal layer. In the lower part the support plates are scratched: the field of view is dark. The upper part is not scratched. We have no extinction.

If the groove spacing is great the liquid crystal is aligned only in the grooves and in the close neighborhood (see Fig. 3).

3. Theory

In the following considerations we assume that the LC molecules, lying parallel to the supporting surface, do not stick to it but may be rotated round the surface normal. As shown above, the rubbing procedure results in a surface deformation. In general this will cause an orientational deformation of the LC. Thus, the homogeneous alignment parallel to the rubbing direction follows directly from the fact that the deformation energy is a minimum in this case.

Consider a sinusoidally shaped surface as shown in Fig. 4. We presume that in the interface the molecules are lying parallel to the surface, but are inclined with respect to the grooves by an angle θ as shown in the figure. The x-axis of our coordinate system is chosen parallel to the mean director, the z-axis is normal to the mean surface and the y-axis completes the right-handed system. The surface now is described by

$$z = a \sin \mathbf{qx}$$

where a is the amplitude of the surface deformation and $\mathbf{qx} = q_1 x + q_2 y$ with $q_1 = q \sin\theta$, $q_2 = -q \cos\theta$ and the spacing $2\pi/q$ of neighbored grooves.

If aq is small compared to unity, there will be only small deviations of the director from its mean direction parallel to the x-axis.

In this case the Frank free energy density g is given by[3]

$$2g = K_{11}(n_{y,y} + n_{z,z})^2 + K_{22}(n_{z,y} - n_{y,z})^2 + K_{33}(n_{y,x}^2 + n_{z,x}^2) - 2(K_{22} + K_{24})(n_{y,y} n_{z,z} - n_{y,z} n_{z,y}) \qquad (1)$$

where Frank's notation of the elastic constants is used and $n_{i,K}$ denotes the derivative of the i-component of the director $\mathbf{n}$ with respect to the coordinate K.

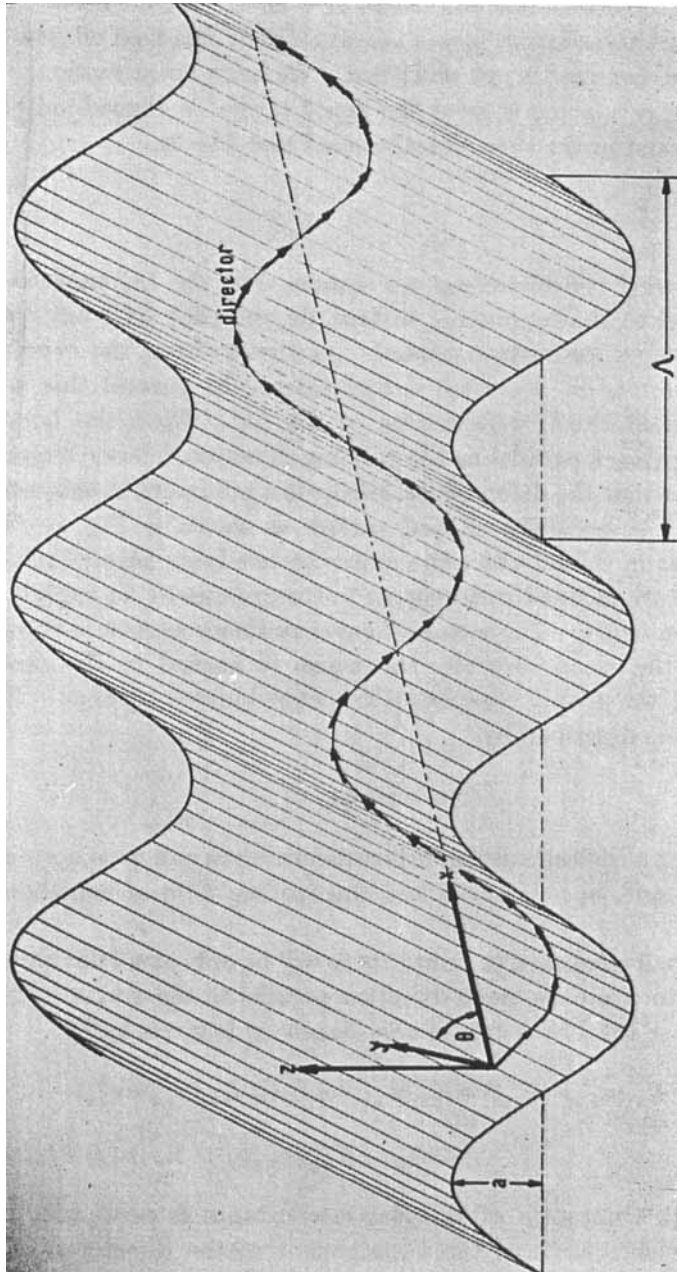

Figure 4. Sinusoidally shaped surface with a deformation amplitude a and a groove-spacing $\Lambda = 2\pi/q$. The director lies in the surface as indicated by the arrows and makes an angle θ with respect to the groove direction.

The equilibrium condition of vanishing couple per unit volume yields[4]

$$\left(\frac{\partial g}{\partial n_{i,K}}\right)_K = 0 \tag{2}$$

or

$$\begin{aligned}(K_{11}-K_{22})n_{z,yz}+K_{33}n_{y,xx}+K_{11}n_{y,yy}+K_{22}n_{y,zz}&=0\\(K_{11}-K_{22})n_{y,yz}+K_{33}n_{z,xx}+K_{22}n_{z,yy}+K_{11}n_{z,zz}&=0\end{aligned} \tag{3}$$

These coupled second order differential equations may be combined to one fourth order equation:

$$[K_{33}\partial_x{}^2+K_{11}(\partial_y{}^2+\partial_z{}^2)][K_{33}\partial_x{}^2+K_{22}(\partial_y{}^2+\partial_z{}^2)]n_z=0 \tag{4}$$

The operators $\partial_i{}^K$ indicate the Kth derivative with respect to the coordinate i. The general solution of (4) is given by

$$\begin{aligned}n_z=f^1(i(p_1x+p_2y)+\gamma_1z)+f^2(i(p_1x+p_2y)+\gamma_2z)\\+g^1(i(p_1x+p_2y)-\gamma_1z)+g^2(i(p_1x+p_2y)-\gamma_2z)\end{aligned} \tag{5}$$

with

$$\gamma_1{}^2=p_2{}^2+p_1{}^2\frac{K_{33}}{K_{22}}\,;\qquad \gamma_2{}^2=p_2{}^2+p_1{}^2\frac{K_{33}}{K_{11}}$$

and with arbitrary constants p_1 and p_2 and arbitrary functions f^1, f^2, g^1 and g^2, which are determined by the boundary conditions.

Since Eq. (1) holds only for small components n_y and n_z, we have to solve Eq. (3) in lowest-order approximation with respect to aq. With this approximation, $n_x=1$; $n_y=0(aq)$; $n_z=0(aq)$ and the boundary conditions which have to be fulfilled are

$$aq_1\cos\mathbf{qx}-n_z\big|_{z=0}=0 \tag{6}$$

(director parallel to the surface), and

$$[K_{22}n_{y,z}+K_{24}n_{z,y}]_{z=0}=0 \tag{7}$$

(vanishing couple stress normal to the surface).

Condition (7) has to be introduced since we assume that the LC molecules may be rotated round the surface normal. For the solution of the problem, two further boundary conditions are necessary. For the sake of simplicity we choose

$$n_y=n_z=0\qquad \text{for } z\to\infty \tag{8}$$

The solutions of Eq. (3) consistent with the boundary conditions (6), (7) and (8) are

$$n_z = \frac{a}{K_{33}q_1}\{-(K_{22}+K_{24})q_2^2\exp(-\gamma_1 z) + [K_{33}q_1^2+(K_{22}+K_{24})q_2^2]\exp(-\gamma_2 z)\}\cos \mathbf{qx}$$

$$n_y = \frac{a}{K_{33}q_1}\left\{-(K_{22}+K_{24})\gamma_1 q_2\exp(-\gamma_1 z) + \frac{q_2}{\gamma_2}[K_{33}q_1^2+(K_{22}+K_{24})q_2^2]\exp(-\gamma_2 z)\right\}\sin \mathbf{qx} \qquad (9)$$

with

$$\gamma_1^2 = \frac{K_{33}}{K_{22}}q_1^2+q_2^2; \qquad \gamma_2^2 = \frac{K_{33}}{K_{11}}q_1^2+q_2^2;$$

and

$$q_1 = q\sin\theta; \qquad q_2 = -q\cos\theta.$$

It is easily seen that $n_y = n_z = 0$ in the limit $q_1 \to 0$ for any z. If the director is parallel to the grooves there is no orientational deformation and hence the energy is minimum, as expected. If the director is inclined with respect to the grooves ($q_1 \neq 0$) then a y-component occurs which is zero on the surface elevations and depressions and is maximum on the points of inflection. The existence of a component n_y on the surface is due to boundary condition (7) (vanishing surface couple stress). This is seen from the surface couple stress normal to the surface, which occurs when the long axes of the molecules are fixed on the surface, i.e. $n_y|_{z=0} = 0$ instead of boundary condition (7). It is given by

$$\left.\frac{\partial g}{\partial n_{y,z}}\right|_{z=0} = aq_1 q_2 \sin \mathbf{qx}\cdot K_{24} \qquad (10)$$

($K_{11} = K_{22}$ for simplicity).

It seems plausible that these counteracting couple forces in the surface depressions and on the surface elevations will no longer be of equal amount, if the condition $aq \ll 1$ is dropped, for then the orientational deformation in the surface depressions will be stronger than on the surface elevations.

Now we want to show that in this case the molecules may not only be rotated into the trivial equilibrium position $q_1 = 0$, but that a

metastable orientation $q_2 = 0$ should also be possible, i.e. an orientation of the molecules perpendicular to the grooves. In order to prove this, we use the solutions (8) to compute the total orientational energy G

$$G = \int_v \mathrm{d}v\, g$$

Knowing that g is a quadratic form of the deformations, we write

$$2g = n_{i,K} \frac{\partial g}{\partial n_{i,K}}$$

and use Eq. (2), and integrate by parts to retain

$$G = \tfrac{1}{2} \oint \mathrm{d}f_K\, n_i \frac{\partial g}{\partial n_{i,K}} = -\tfrac{1}{2} \int_{z=0} \mathrm{d}x\, \mathrm{d}y\, n_i \frac{\partial g}{\partial n_{i,z}}$$

By replacing the integral by the average over x and y, and using Eq. 7, we get the energy per unit area

$$\rho = -\tfrac{1}{2}(K_{11} - K_{22} - K_{24})\, \overline{n_z n_{y,y}} - \tfrac{1}{2} K_{11}\, \overline{n_z n_{z,z}}$$

where the bars denote the average.

We use Eq. (9) and compute the first and second derivative with respect to θ at $\theta = \pi/2$. The first derivative vanishes, indicating an extremal value of the energy. It is a minimum if the second derivative is positive. This is the case if

$$(K_{22} + K_{24})\left(2 - \frac{K_{22} + K_{24}}{\sqrt{K_{11} K_{22}}}\right) > \tfrac{1}{2}(K_{11} + 3K_{33}) \qquad (11)$$

This inequality is not easily understandable. Therefore we will give the corresponding inequality in the case of fixed director on the surface ($n_y \big|_{z=0} = 0$ instead of boundary condition (7)):

$$K_{22} > 3K_{33} \qquad (K_{11} = K_{22} \text{ for simplicity}). \qquad (12)$$

It is easy to make this inequality plausible. Let the director be inclined to the groove direction. Then the orientation pattern comprises twist. If the director is perpendicular to the grooves, the orientation is strongly bent. If the molecules are rotated out of this direction twist energy will increase and bent energy will decrease. Thus, if the ratio of twist to bent constant is sufficiently large, the alignment perpendicular to the grooves will be metastable.

Now one can argue in a similar way for the case of the correct boundary condition. The main difference is that by rotation of the molecules the twist may be partly transformed into other types of deformation. Therefore inequality (11) has a more complex form.

4. Concluding Remarks

In our theoretical approach we neglected the natural surface roughness of the substrate material. Therefore it is limited to cases where the micro-grooves induced by rubbing predominate over the surface roughness. For many materials this will be contradictory to our assumption of small surface deformations. Therefore our results are only qualitatively applicable.

Concerning the observation of the metastable alignment perpendicular to the grooves, we want to suggest the following experiment: Strong field induced hydrodynamic turbulence may detach the LC molecules from the supporting surface. After abruptly switching off the electrical field, areas of metastable alignment should be observable in a LC with the proper elastic constants. First experiments of our own are encouraging, though the interpretation is not unique at present.

We have shown that the orientational deformation energy due to surface deformations is responsible for the homogeneous alignment of the LC parallel to the substrate. It should be mentioned that other types of alignment may be explained by similar arguments. For example, if the interaction between substrate and LC favors a homeotropic alignment, micro-grooves will lead to splay deformation near the surface. The total energy may be reduced by uniform tilt of the layer in groove direction, in agreement with experimental observations.

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