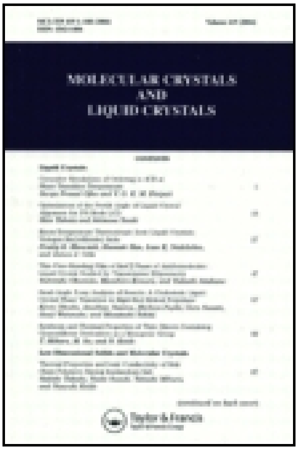

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Coupling Between Nematic Liquid Crystals and Treated Substrates for a Pure Twist Deformation: A Computer Simulation

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Version of record first published: 21 Mar 2007.

To cite this article: M. Ide , T. Oh-ide & S. Kobayashi (1987): Coupling Between Nematic Liquid Crystals and Treated Substrates for a Pure Twist Deformation: A Computer Simulation, Molecular Crystals and Liquid Crystals, 144:5, 225-234

To link to this article: http://dx.doi.org/10.1080/15421408708084217

Mol. Cryst. Liq. Cryst., 1987, Vol. 144, pp. 225–234
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Coupling Between Nematic Liquid Crystals and Treated Substrates for a Pure Twist Deformation: A Computer Simulation†

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(*Received August 22, 1986; in final form September 12, 1986*)

The result of a computer simulation of an optical detection of the coupling strengths of surface coupling of nematic liquid crystals (NLC) subjected to pure twist is described. Transmitted light beams through the homogeneously aligned NLC medium sandwiched between crossed polarizers are calculated. The LC medium is subjected to a pure twist by the application of magnetic fields. The medium has to be adjusted to have 180 degrees phase retardation prior to the application of the magnetic field; this assures a zero transmission for the magnetic field even above the threshold. The movement of the molecules in the vicinity of the surface will be detected by rotating polarizers so as to keep the transmitted light to zero. The torsional coupling constant will be evaluated by searching zero transmitted light by the rotation of the polarizers.

Keywords: surface anchoring, torsional deformation

INTRODUCTION

Preparation of a monodomain liquid crystal medium with a fairly large area is inevitable and necessary to extend fundamental and practical research work on liquid crystals. This process relies on the surface alignment of liquid crystals. There exist two kinds of director changes in the vicinity of the surface due to the application of external

†Presented at the 11th International Liquid Crystal Conference, June 30–July 4, 1986, Berkeley, CA U.S.A.

forces; one is the polar deformation which causes the change in the angle between the director and the normal to the sample. The other is the azimuthal deformation or torsional (pure twist) motion of molecules in the plane of the sample. A great deal of work has been devoted to the former, both in the deformation in planar conformation[1,2] and the homeotropic ones,[1,3,4] but only a few papers on the anchoring strength for pure twist deformation have been published.[5,6] Nevertheless, its importance was pointed out in a published paper.[7]

From the threshold magnetic field for the pure twist deformation one can determine the coupling strength. However, this method is useful only for a thick sample, say 100 μm thick, where the extrapolating length is negligible. Moreover, it is hard to determine an accurate threshold field because of critical slowing down phenomena occurring in the Freedericksz transition; it is necessary to scan the field at very low rate. This difficulty can be resolved by observing a wide range of the deformation of an LC medium caused by applied fields ranging from zero to far above the threshold.

Several measuring methods of the pure twist deformation have been proposed;[8,9] among them the approach taken by Gerber and Schadt,[9] which was developed originally for determining the twist elastic constant, seems practical because it relies on the zero transmitted light intensity that promises high accuracy in the measurement. Another possibility is to use a tunable birefringent effect for obliquely incident light, with which one can determine the threshold field, but it needs a precise curve fitting to the transmitted light intensity.

In this work, a computer simulation was performed to evaluate the magnitude of the rotation angle of the director at the boundary surface in a homogeneously aligned nematic cell subjected to a pure twist deformation by the application of a magnetic field, and to evaluate the torsional surface coupling strength.

OBJECTIVE SYSTEM

In Figure 1 the system consisting of the sample and the optical detection system is shown. The NLC is homogeneously aligned and sandwiched between a pair of crossed polarizers so as to shut the transmitted light in a zero field.

The direction of the incident light is normal to the sample and this makes the system simple. Each polarizer can be rotated independently so as to control the intensity of the transmitted light through the system.

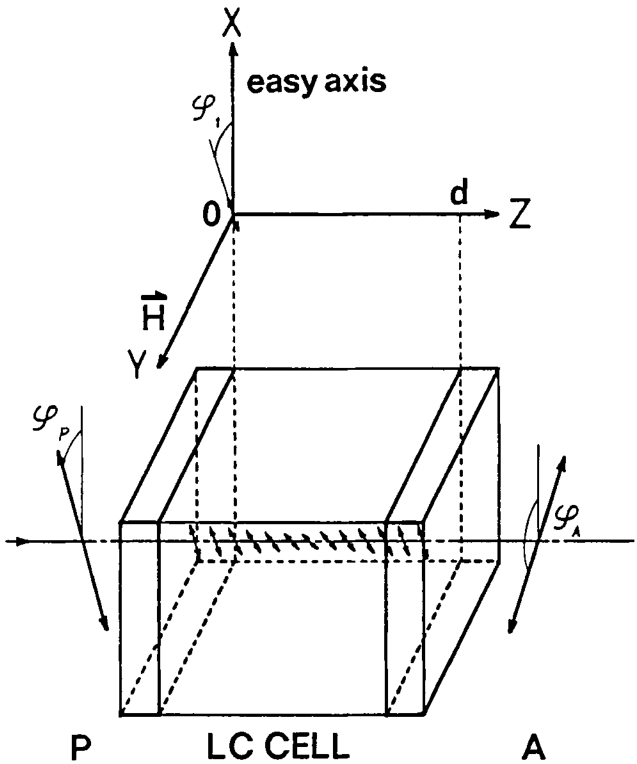

FIGURE 1 The sample medium, direction of the applied magnetic field, and optical system.

APPROXIMATE ANALYTICAL EXPRESSION

After some manipulations of the equation given by Gerber and Schadt[9] one obtains a formula for the transmitted light as:

$$I = \frac{\pi}{d}\left(\frac{n_e}{n_0}\right)\frac{1}{\delta q + \pi/d} E_1^2 \cdot \varphi_m^2 \,(1+\cos\Delta) \tag{1}$$

where d, n_e, n_0, E_1 and φ_m are the thickness of the LC medium, the refractive index for the extraordinary ray, that for the ordinary ray, the amplitude of the optical field, the twist angle of the director at the mid plane, and

$$\delta q = \frac{2\pi}{\lambda_0}(n_e - n_0)$$

and further Δ reads

$$\Delta = \delta q \cdot d$$

which is the phase retardation.

An approximate value for a light intensity for $\Delta = 2\pi$ is given from Eq. (1) as

$$I = 2C_1^2(H-H_c)/H_c \qquad (2)$$

where C_1^2 is the proportional constant, and an approximate formula for φ_m, $\varphi_m^2 = (H-Hc)/Hc$, is used, where H_c is the threshold magnetic field. This condition was used to determine K_2.[9]

We are interested in the case where $I = 0$, even though H exceeds H_c, until the adiabatic condition is destroyed.

When the surface anchoring is weak or the thickness of the LC medium is small, even for $\Delta = \pi$, it is expected to be able to observe a leak of the light caused by the rotation of the directors close to the surface boundaries at $H > H_c$. However, this leak can be reduced substantially (to zero) by the appropriate rotation of the polarizers. The amount of the rotation of the polarizers is thought to be the rotation angle of the director at the surfaces.

This value gives a measure of the coupling strength, but the accurate determination of it is left to more detailed analysis based on the computer simulation described in the following section.

COMPUTER SIMULATION

The treatment of the light propagation in an optically anisotropic medium such as LC is well achieved by using the 4×4 matrix method.[10] In this work, in order to save computation time, we used a simplified one, called the 2×2 method,[11] in which the reflected ray from the LC medium can be safely ignored since the distortion of the medium is not so large.

For light propagating in the free space with wavevector k, we chose a coordinate system so that $k_y = 0$ (see Figure 2). In this coordinate system, the electromagnetic vectors in the liquid crystal layer can be written as:

$$\vec{E} = \vec{E}(z)\exp[i(kx\sin\theta - \omega t)] \qquad (3)$$

$$\vec{H} = \vec{H}(z)\exp[i(kx\sin\theta - \omega t)] \qquad (4)$$

where θ is the incidence angle in the air.

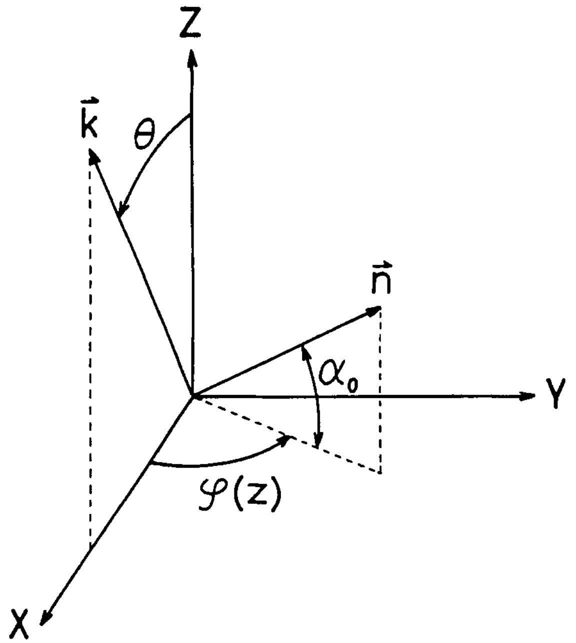

FIGURE 2 The definitions of the angles relevant to the direction of the k-vector of the incident light and that of the nematic medium.

Vectors E and H satisfy Maxwell's equations:

$$\operatorname{div} \vec{D} = 0 \tag{5}$$

$$\operatorname{div} \vec{B} = 0 \tag{6}$$

$$-i\frac{c}{\omega}\frac{\partial}{\partial z}\begin{bmatrix} E_x \\ E_y \\ H_x \\ H_y \end{bmatrix} = \begin{bmatrix} -\dfrac{\epsilon_{xz}}{\epsilon_{zz}}X, & -\dfrac{\epsilon_{yz}}{\epsilon_{zz}}X, & 0, & 1-\dfrac{1}{\epsilon_{zz}}X^2 \\ 0, & 0, & -1, & 0 \\ \dfrac{\epsilon_{xz}\epsilon_{yz}}{\epsilon_{zz}}-\epsilon_{xy}, & X^2+\dfrac{\epsilon_{yz}^2}{\epsilon_{zz}}-\epsilon_{yy} & 0, & \dfrac{\epsilon_{yz}}{\epsilon_{zz}}X \\ \epsilon_{xx}-\dfrac{\epsilon_{xz}^2}{\epsilon_{zz}}, & \epsilon_{xy}-\dfrac{\epsilon_{xz}\epsilon_{yz}}{\epsilon_{zz}}, & 0, & -\dfrac{\epsilon_{xz}}{\epsilon_{zz}}X \end{bmatrix}\begin{bmatrix} Ex \\ Ey \\ Hx \\ Hy \end{bmatrix}$$

$$\equiv A\,\vec{x} \tag{7}$$

$$\frac{\partial}{\partial z}\vec{x} = i\frac{\omega}{c}A\,\vec{x} \tag{8}$$

where

$$X = \sin\theta$$

$$\epsilon_{xx} = \epsilon_2 + (\epsilon_1 - \epsilon_2)\cos^2\alpha_0\cos^2\varphi$$

$$\epsilon_{yy} = \epsilon_2 + (\epsilon_1 - \epsilon_2)\cos^2\alpha_0\sin^2\varphi$$

$$\epsilon_{zz} = \epsilon_2 + (\epsilon_1 - \epsilon_2)\sin^2\alpha_0$$

$$\epsilon_{xy} = (\epsilon_1 - \epsilon_2)\cos^2\alpha_0\sin\varphi\cos\varphi$$

$$\epsilon_{xz} = (\epsilon_1 - \epsilon_2)\sin\alpha_0\cos\alpha_0\cos\varphi$$

$$\epsilon_{zz} = (\epsilon_1 - \epsilon_2)\sin\alpha_0\cos\alpha_0\sin\varphi$$

and the director twist angle φ is measured from the incidence plane. If the derivative matrix A is a constant, then Eq. (7) has a solution of the form

$$\bar{x}(z + \Delta z) = \exp\left[i\frac{\omega}{c}A\Delta z\right]\bar{x}(z) \tag{9}$$

If the LC layer is divided into several slabs, each with a constant derivative matrix, then

$$\bar{x}(d) = \exp\left[i\frac{\omega}{c}A(d-h)h\right]. \dots\dots\dots \exp\left[i\frac{\omega}{c}A(0)h\right]\bar{x}(0)$$

$$\equiv F\bar{x}(0) \tag{10}$$

where h is the slab thickness. F is the propagator matrix. The division of the liquid crystal layer into slabs of equal thickness would be inefficient as the derivative matrix in Eq. (7) depends on angles rather than distance. It is thus better to change the variable in Eq. (7) from z to λ. A new variable λ, so that

$$\sin\lambda = \frac{\sin\varphi}{\sin\varphi_m}, \tag{11}$$

where φ ($=\varphi(z)$) is the spatial variation of the torsional angle which is obtained by solving a differential equation for the elastic deformation of the medium under the application of a magnetic field.

Further, φ_m stands for the φ at the mid plane of the medium (z = $d/2$). The coupling constant A_φ is introduced in a formula for the surface energy as

$$f_s = 1/2\, A_\varphi \sin^2\varphi_1. \tag{12}$$

Eq. (10) was transformed into

$$\begin{aligned} F = P(\Delta\lambda/2,\Delta\lambda) \cdot P(\lambda_1+\Delta\lambda/2,\Delta\lambda) \ldots\ldots\ldots P(\pi/2-\lambda_n/2,\Delta\lambda) \\ \cdot P(\pi/2-\lambda_n/2,\Delta\lambda) \ldots\ldots\ldots P(\lambda_1+\Delta\lambda/2,\Delta\lambda) \cdot P(\Delta\lambda/2,\Delta\lambda) \end{aligned} \tag{13}$$

where $P(\lambda,\Delta\lambda)$ is the local propagator matrix.

The derivative matrix of Eq. (7) has four eigenvalues:

$$q_{1,2} = \pm\sqrt{\epsilon_2 - X^2} \tag{14}$$

$$q_{3,4} = \frac{1}{\epsilon_2+(\epsilon_1-\epsilon_2)\sin^2\alpha_0}\left[-(\epsilon_1-\epsilon_2)\sin\alpha_0\cos\alpha_0\cos\varphi \cdot X \pm\sqrt{\epsilon_1\epsilon_2\sqrt{\epsilon_2+(\epsilon_1-\epsilon_2)\sin^2\alpha_0 - X^2\left(1-\left(1-\frac{\epsilon_2}{\epsilon_1}\right)\cos^2\alpha_0\sin^2\varphi\right)}}\right] \tag{15}$$

corresponding to the ordinary and extraordinary transmitted and reflected waves.

Since at the magnetic field intensity with which we are concerned there are no abrupt changes either in the indices of refraction or in the structure ($\partial\varphi/\partial z << 1/d$), we can safely neglect the reflected waves and solve Eq. (7) for transmitted waves only. This transforms Eq. (7) into a 2×2 differential matrix equation.

Then, it is enough to take only two eigenvalues, q_1 and q_3 (with a positive sign), from the four given by Eq. (14) and (15). Thus, the tensor equation becomes

$$T^{-1} A \, T = \begin{bmatrix} q_1 & 0 \\ 0 & q_3 \end{bmatrix} \tag{16}$$

where T is the tensor whose components are eigenvectors.

As a result the local propagator matrix by the eigenvectors is given by

$$P(\lambda,\Delta\lambda) = T \begin{bmatrix} \exp[i\frac{\omega}{c}\, q_1 \frac{\partial z}{\partial \lambda} \Delta\lambda] & 0 \\ 0 & \exp[i\frac{\omega}{c}\, q_3 \frac{\partial z}{\partial \lambda} \Delta\lambda] \end{bmatrix} T^{-1} \tag{17}$$

Thus, using Eq. (16) one can calculate the transmitted light through the deformed medium.

RESULTS AND DISCUSSION

Figure 3 shows the result of the computer simulation of the transmitted light versus the applied magnetic field. The assumed LC is MBBA since its material parameters are relatively well known. In

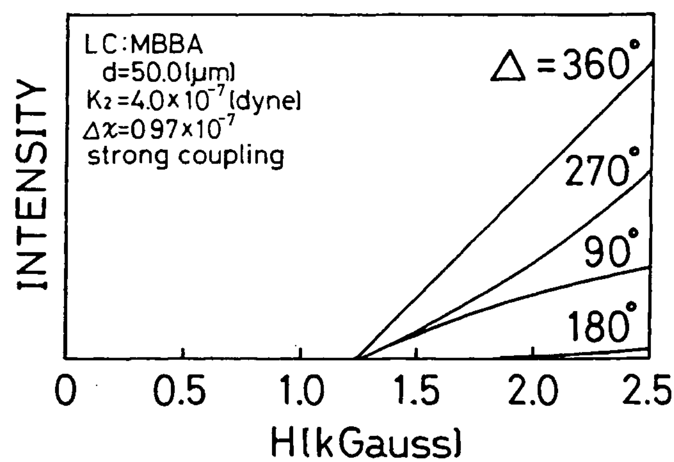

FIGURE 3 Result of the computer simulation for the transmitted light intensity vs. magnetic field. MBBA is taken as sample, and strong coupling is assumed.

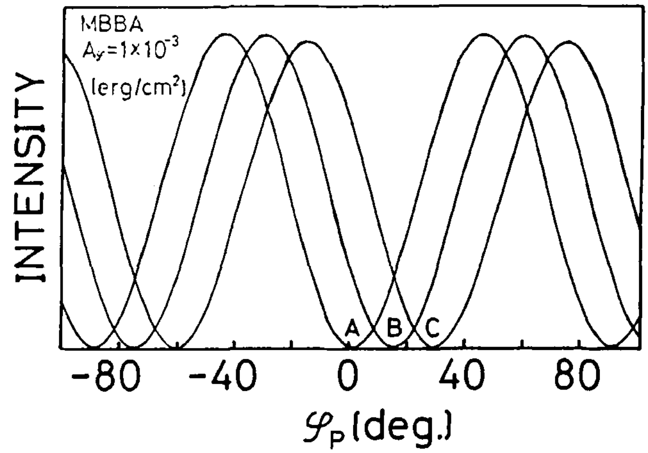

FIGURE 4 Result of the computer simulation of the optical effect in a sample with weak surface coupling. The ordinate is the transmitted light intensity, abscissa is the setting angle of the polarizers under various magnetic fields; A, 1.1[kG]; B, 1.5[kG]; and C, 2.5[kG].

these calculations we assumed strong coupling. For $\Delta = 2\pi$, a straight line starting from the H_c point is obtained. This behavior agrees fairly well with the prediction given by Eq. (2). For $\Delta = \pi$, zero transmitted light is obtained even at $H > H_c$.

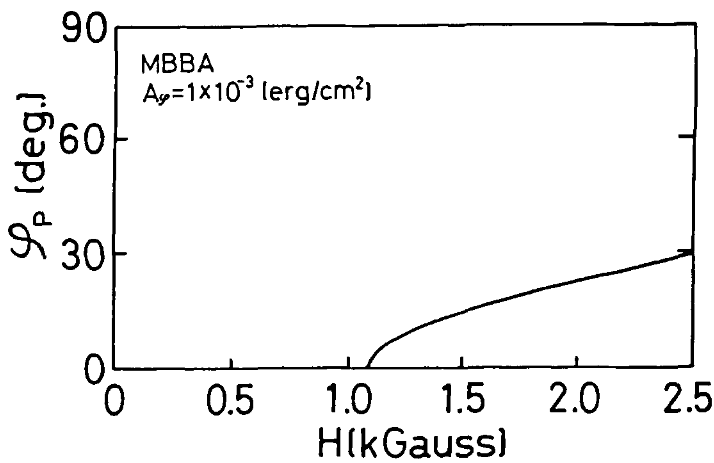

FIGURE 5 Setting angles of the polarizers necessary to keep zero transmitted light vs. applied magnetic field.

Then we explored the case of weak coupling. We assumed 1×10^{-3} erg/cm^2 as the torsional coupling constant.

Figure 4 shows the result of computer simulation for the intensity of the transmitted light versus the rotation angle of the polarizers. In this figure the parameters are the applied magnetic fields; from these curves we searched for the condition giving rise to $I = 0$.

Figure 5 gives the necessary rotation angle, which is taken from the more detailed calculation that is shown in Figure 4 to keep zero transmitted light when A_φ is given as above.

It is estimated that the necessary rotation angle of the polarizers reaches 10 to 20 degrees for the assumed torsional coupling constant. The measurement and determination of the torsional coupling constant seem possible with fairly good accuracy. Actual measurement is now under way and the result will be published in the near future.

Acknowledgment

Stimulating discussion with H. Birecki is gratefully acknowledged.

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