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Optical method for determining anisotropy of diamagnetic susceptibility of nematics and polar anchoring energy coefficient of nematics-substrate systems by using a cell of varying thickness

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A wedge cell of the wedge angle of the order of few milliradians was used to measure threshold magnetic fields for the magnetic Fréedericksz transition [1–3]. A nematic liquid crystal filling the cell was of planar orientation enforced by the treatment of the flat boundary plates. A system of interference fringes appeared in the cell placed in normally incident light between analyser and polariser crossed. In the vicinity of each fringe, the cell could be considered as a flat-parallel one and hence it was equivalent to a system of flat cells of different precisely determined thickness, the same relates to any cell of slowly-varying thickness and flat cover plates. The threshold magnetic field magnitudes were interpreted as eigenvalues of the boundary eigenvalue problem for the operator of the second derivative; the interaction between the nematics and the substrate was described by the Rapini-Papoular formula [3] (i.e., weak coupling was considered). The resulting formulae were used to determine the polar anchoring energy coefficient and the anisotropy of diamagnetic susceptibility after the threshold fields measured. The method was applied to characterise the nematic liquid crystal 5CB and the coupling between it and the substrates made of poly(amic acid) MP2 [4,5]. The estimates of material parameters agreed pretty well with those determined by the composite method [6].

Keywords: nematics elastic constants, magnetic susceptibility anisotropy, 4'-pentyl-4-cyanobipfenyl (5CB), polar anchoring energy coefficient, wedge cell method.

1. Introduction

Some material parameters of nematic liquid crystals, like elastic constants and anisotropy of diamagnetic susceptibility, cannot be measured immediately. A possible way for determining them is to find their values by comparing results of measurements of optical response of a nematic liquid crystal cell with results of computer simulations based on an adequate mathematical model. The quantity frequently used as monitoring the director field inside a flat nematic cell is the phase shift between the ordinary and extraordinary rays of coherent light beam normally incident on the cell. The scheme of the measurement system for recording the optical response of a cell to external electric or magnetic field is shown in Fig. 1.

For more reliable estimation of the material parameter magnitudes it is necessary to dispose of results of measurements done with several cells with the same treatment of

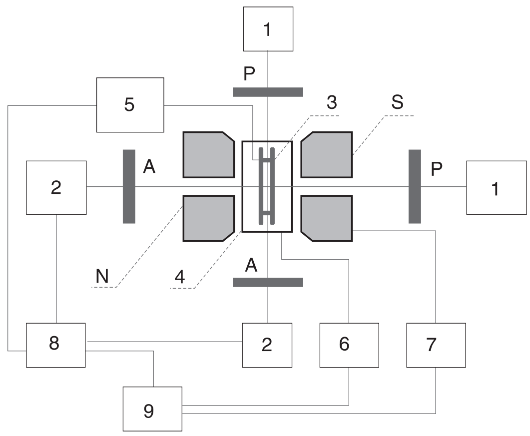

Fig. 1. Block diagram of the measurement system for studying nematics deformations in magnetic and electric fields: 1 – He-Ne laser, 2 – projection objective, 3 – liquid crystal cell, 4 – thermostatic measuring chamber, 5 – RLC bridge or function generator, 6 – thermo-stabiliser, 7 – electro-magnet power supply control device with magnetic field intensity measuring unit, 8 – microscope with photodetector and digital voltmeter, 9 – computer system with the IEEE 488 bus for recording results, A – analyser, P – polariser.

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the cell cover coatings. A cell of slowly varying thickness may substitute several flat-parallel cells in such experiments. A wedge cell, used in experiments presented in this article, is an example of such a cell.

A wedge nematics cell was made of glass plates (size 22×35 mm), coated with indium-tin oxide electrodes and orienting layer of polyimide MP2 – poly(amic acid) [4,5], polymerised and then rubbed. The plates were glued without a spacer along one edge and with a spacer (of thickness about 200 μm) along the other. The orientation of the nematics molecules enforced by substrates was parallel to the boundaries and to the wedge edge. The cell was placed in a thermostatic stage between the polariser and analyser crossed in the measurement system, consisting of a He-Ne laser and a microscope with a photodetector, and between pole pieces of an electromagnet, as in Fig. 1. In the normally incident light, a system of interference fringes appeared, as in schematic Fig. 2. In the small neighbourhood of each fringe position a wedge cell can be treated as the planar one (like sketched in Fig. 3) due to a very small wedge angle. In such experiment, a wedge cell is equivalent to a system of planar cells of different thickness.

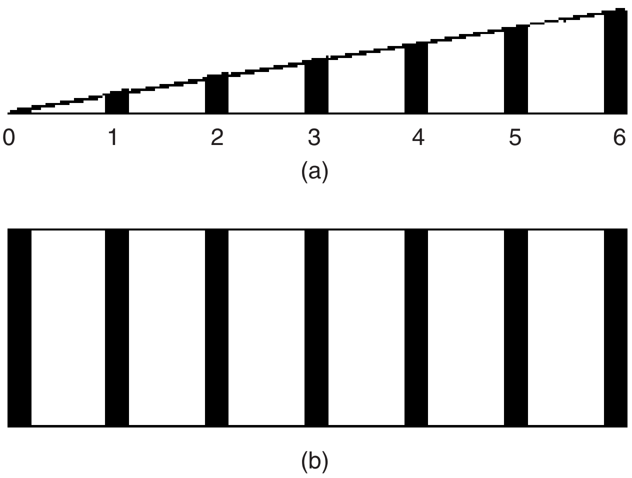

Fig. 2. System of interference fringes of normally incident light in a wedge cell, filled with a nematics of planar alignment, in the absence of external fields: $\Phi_j = 2\pi\Delta_j\lambda^{-1}$, $d_j = \Delta_j n_a^{-1}$, $n_a \equiv n_e - n_o$, $\Delta_j = j\lambda$, where j is the order of an interference minimum (displayed in the figure), d is the corresponding cell thickness, Δ is the difference of optical paths, Φ is the phase shift; (a) denotes the side view and (b) denotes the top view.

2. Planar cell locally equivalent to varying-thickness cell

A planar nematics cell is considered as the nematics layer of the thickness d, infinitely extended in the directions Ox and Oy (Fig. 3). It has a basic stationary state of homogeneous director field parallel to the boundaries (i.e. planar alignment), enforced by the plates coated

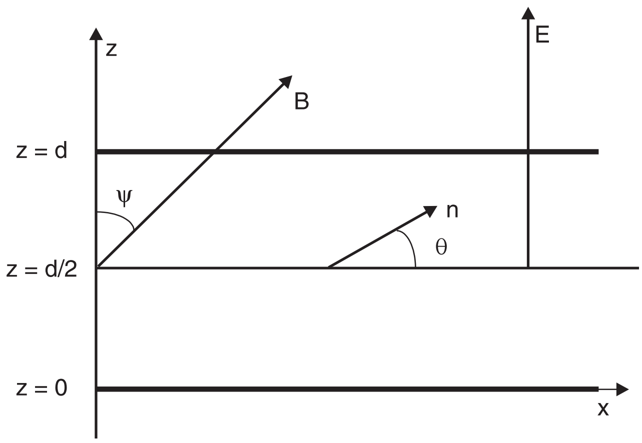

Fig. 3. Sketch of experimental configuration of a flat-parallel nematics cell in external fields. The director, Oz axis and external (magnetic or electric) field vectors are all in the same plane. The one-dimensional approximation is considered, i.e., physical quantities are assumed as depending only on z e.g.: $\vec{n}(z) = (\cos\vartheta(z), 0, \sin\vartheta(z))$, $\vec{E}(z) = (0, 0, E(z))$, $\vec{B}(z) = (B\sin\psi, 0, B\cos\psi)$.

with specially treated substrate. Stationary states of the cell, enforced by a constant magnetic field only, acting perpendicularly or parallel ($\psi = 0$ or $\psi = 1/2\pi$) to the nematics layer in the plane of alignment, can be described in one-dimensional approximation by a planar director field $n = [\cos\vartheta(z), 0, \sin\vartheta(z)]$ characterised by the tilt angle (Fig. 3).

If the surface free energy density on both covers is in accordance with the Rapini-Papoular formula

$$f_s(\vartheta_s) = \frac{1}{2} W \sin^2(\vartheta_s - \vartheta_0), \qquad (1)$$
$$\vartheta_s \equiv \vartheta(0) \quad \text{or} \quad \vartheta_s \equiv \vartheta(d),$$

then the free energy functional for the cell is following

$$\begin{aligned} F(\vartheta(z), \vartheta'(z)) = \\ = \frac{1}{2}\int_0^d [(K_{11}\cos^2\vartheta(z) + K_{33}\sin^2\vartheta'(z))^2]dz \\ - \frac{1}{2}\int_0^d \frac{\chi_a B^2}{\mu_0}\sin^2(\vartheta(z) + \psi)dz \qquad (2) \\ + \frac{1}{2} W \sin^2(\vartheta(0) - \vartheta_0) \\ + \frac{1}{2} W \sin^2(\vartheta(d) - \vartheta_0), \end{aligned}$$

where W is the polar anchoring energy coefficient, ϑ_o is the tilt angle of the minimal-free-energy orientation (i.e., the anchoring direction) at the boundaries, K_{11} and K_{33} are the splay and bend elastic constants, respectively, and χ_a is the anisotropy of diamagnetic susceptibility. The Euler-Lagrange equation takes the form of a system of equations

$$\begin{aligned}&[K_{11}\cos^2\vartheta(z)+K_{33}\sin^2\vartheta(z)]\vartheta''(z)+(K_{33}-K_{11})\sin\vartheta(z)\cos\vartheta(z)(\vartheta'(z))^2\\&+\chi_a\mu_0^{-1}B^2\sin(\vartheta(z)+\psi)\cos(\vartheta(z)+\psi)=0\quad\text{for}\quad 0<z<d,\\&-[K_{11}\cos^2\vartheta(0)+K_{33}\sin^2\vartheta(0)]\vartheta'(0)+W\sin(\vartheta(0)-\vartheta_0)\cos(\vartheta(0)-\vartheta_0)=0,\\&[K_{11}\cos^2\vartheta(d)+K_{33}\sin^2\vartheta(d)]\vartheta'(d)+W\sin(\vartheta(d)-\vartheta_0)\cos(\vartheta(d)-\vartheta_0)=0.\end{aligned}\qquad(3)$$

The stationary states of a cell with a nematics of positive anisotropy of diamagnetic susceptibility ($\chi_a > 0$), corresponding to weak magnetic fields acting perpendicularly to the layer $\psi = 0$ and small deformations, can be described by a linearised version of the Euler-Lagrange equations; if $\vartheta_o = 0$ and $\vartheta \approx 0$ then $\sin\vartheta \approx \vartheta$, $\cos\vartheta \approx 1$ and

$$\begin{aligned}&K_{11}\vartheta''(z)+\mu_0^{-1}\chi_a B^2\vartheta(z)=0\quad\text{for}\quad 0<z<d,\\&K_{11}\vartheta'(0)-W\vartheta(0)=0,\\&K_{11}\vartheta'(d)-W\vartheta(d)=0.\end{aligned}\qquad(4)$$

This system has a solution of the form $\vartheta(z) = C_1\cos\omega z + C_2\sin\omega z$, being a solution of the first equation with $\omega^2 \equiv \mu_0^{-1}\chi_a B^2 K_{11}^{-1}$ and the constants C_1 and C_2 satisfying the two other equations. This implies the condition for the stability of the basic stationary state [2], it is stable until magnetic field is greater than the Fréedericksz threshold for the weak anchoring B_w, being the smallest root of the characteristic equation

$$\frac{\sqrt{\mu_0^{-1}\chi_a K_{11}}}{Wd}B_w d=\cot\left(\frac{1}{2}\sqrt{\frac{\chi_a}{\mu_0 K_{11}}}B_w d\right).\qquad(5)$$

The last equation can be written in the following form, in which both sides depend linearly on the cell thickness d

$$\begin{aligned}Wd&=\sqrt{\mu_0^{-1}\chi_a K_{11}}B_w d\tan\left(\frac{1}{2}\sqrt{\frac{\chi_a}{\mu_0 K_{11}}}B_w d\right)\\&\equiv f_w(\chi_a,K_{11};B_w d).\end{aligned}\qquad(6)$$

The polar anchoring energy coefficient W can be calculated from this equation after the dependence of the magnetic tension $B_w d$ on the cell thickness d, for the values of other parameters, K_{11} and χ_a, given. Moreover, it is observed that the curve $f_w(d)$ is not linear for the given set of B_w and d measured unless both parameters K_{11} and χ_a have the proper values; this can be exploited to determine both W and one of the parameters K_{11} or χ_a simultaneously (given the other). These dependencies are presented by example of the obtained results in Fig. 7. It should be emphasised that the accuracy of determining the material constants of nematics (K_{11} or χ_a) and nematics-substrate systems (W) is limited by assumptions made to obtain the last formula: the anchoring of nematics molecules at the boundaries being in accordance with the Rapini-Papoular formula and the anchoring direction being equal to zero.

3. Results of measurements and computations

The intensity of normally incident light transmitted through the cell in the positions of selected interference fringes was recorded as a function of applied magnetic field (Fig. 4). The phase shift between ordinary and extraordinary rays as a function of a magnetic field was calculated from each of such characteristics by finding positions of subsequent maxima and minima (Fig. 5). The threshold field for the Fréedericksz transition was determined by linear extrapolation from the first four extremes. The procedure was applied for interference fringes from 6th to 11th.

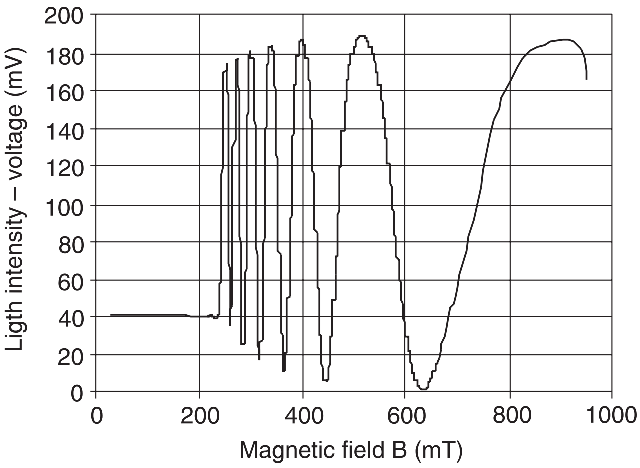

Fig. 4. Changes of the intensity of light transmitted through a nematics wedge cell in the place of the appearance of eighth interference fringe (for system 5CB – MP2) with magnetic field applied (for example).

The magnitudes of the polar anchoring energy coefficient W and the anisotropy of diamagnetic susceptibility χ_a were found as solution of Eq. (6) by non-linear least-square fitting of the value of χ_a, with using the values of magnetic tension experimentally determined as a function of cell thickness, to obtain the best linear approximation of function f_w and calculating W as the slope of this direct line (Fig. 7, given K_{11}). Good agreement of simulated and measured values of magnetic tension was achieved (Fig. 6).

The values of the three parameters, determined by more accurate method [6] at the temperature 22.7°C, were following: $\chi_a = 1.56\times10^{-6}$, $K_{11} = 6.47$ pN, $W = 18.7$ μJm^{-2}; the magnitude W was estimated by linear extrapolation of the non-linear dependence of the boundary value of the tilt angle, $\vartheta(0) = \vartheta(d)$, on the boundary value of the elas-

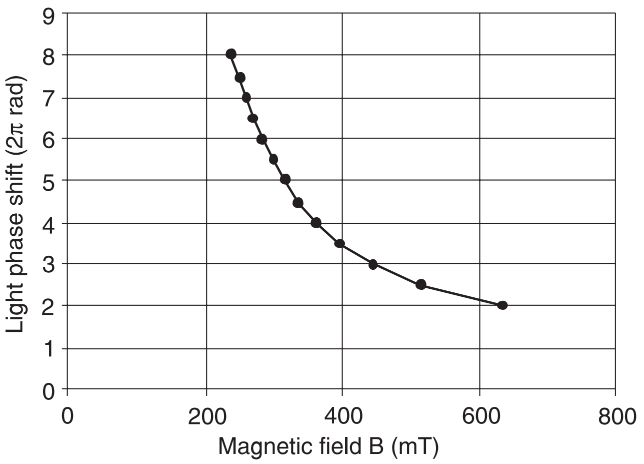

Fig. 5. Phase shift corresponding to subsequent extreme points of the curve in Fig. 4 as a function of applied magnetic field; the Fréedericksz threshold field for weak anchoring is determined as corresponding to that of the biggest shift (i.e. zero-order minimum) found by linear extrapolation from subsequent four extreme points (this part of the curve is linear).

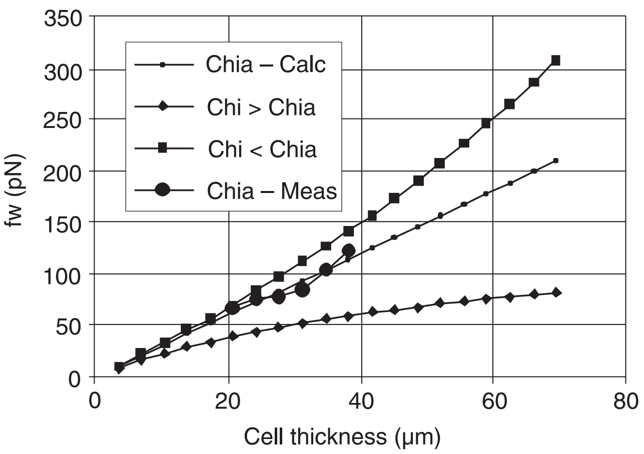

Fig. 7. Right-hand-side of the main formula calculated for threshold magnetic fields measured, corresponding to seven cell thickness (i.e. the interference fringes from 6th to 11th corresponding to cell thickness 20.9÷38.2 µm), and simulated, by using the magnitudes W = 3.01 µJm^{-2} and χ_a = 1.44×10^{-6} from fitting with assumed K_{11} = 7.07 pN. The two additional curves show the values of this function corresponding to the same values of all parameters except of χ_a taken greater or smaller than the former one obtained from fitting procedure.

tic torque density [6]. Using this method one obtains χ_a = 1.56×10^{-6}, W = 3.27 µJm^{-2} by taking K_{11} = 7.67 pN or χ_a = 1.32×10^{-6}, W = 2.76 µJm^{-2} by taking K_{11} = 6.47 pN, or W = 3.01 µJm^{-2} and χ_a = 1.44×10^{-6} by taking K_{11} = 7.07 pN (as referred to in Fig. 7), all results with the same precision of fitting the function f_w by a linear function. It illustrates possible accuracy of the method. The differences may be attributed mostly to inaccuracy of determining the positions of extreme points of transmitted light intensity (up to about 3 mT) and to inaccuracy of determining the temperature of the measurement stage (within 0.2°C). The disagreement between the magnitudes of the polar anchoring energy coefficient, obtained by the method presented here and by more complicated one [6] can be attributed to the lack of values of the light phase shift on the magnetic field corresponding to the field magnitudes close to the threshold one, what features the procedure applied for determining them [6], and moreover to the influence of non-zero anchoring angle (about 0.0082 rad).

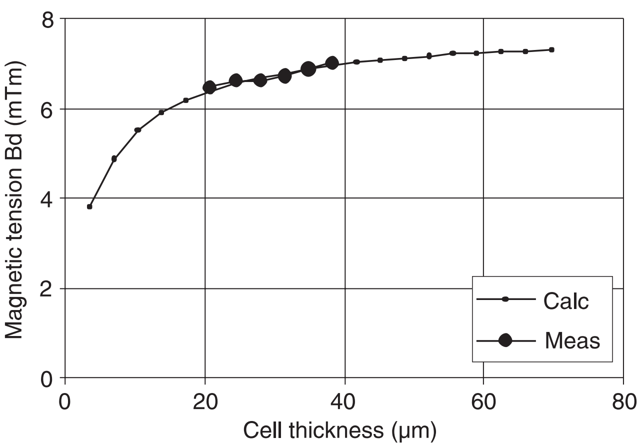

Fig. 6. Magnetic tension as a function of cell thickness, measured and calculated by using values of W and χ_a from fitting (the same as in Fig. 7).

4. Conclusions

The experimental and computational method presented above is a good procedure for a first-look estimation of the polar anchoring energy coefficient for nematics-substrate systems and (simultaneously) one of the nematics material constants, the anisotropy of diamagnetic susceptibility or the splay elastic constant. The computational method can be also exploited with the use of threshold magnetic fields determined for a set of flat-parallel cells of different thickness, but the use of a wedge cell takes advantage of uniformity of boundary conditions and accuracy of determining the cell thickness.

The method can be used only in the case of weak anchoring (when the polar anchoring energy coefficient is of the order of 1 µJm^{-2}, as above). Moreover, due to very small differences between the values of threshold magnetic tension corresponding to larger cell thickness (see Fig. 6), one can obtain more reliable estimates of the magnitudes of material parameters using results of measurements for smaller cell thickness.

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