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Experimental Study of Anchoring Characteristics and Splay-Bend Surface-Like Elasticity of Nematics with Using Non-Twisted Nematic Cells

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### Experimental Study of Anchoring Characteristics and Splay-Bend Surface-Like Elasticity of Nematics with Using Non-Twisted Nematic Cells

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Question of second-order terms in bulk elastic free energy functional for nematics is discussed and investigated experimentally. Under assumption that these surface-like terms contribute only to surface free energy functional, they were firstly substituted by boundary conditions. Several flat-parallel cells (of thickness from 1.9 µm to 31.2 µm) filled with 5CB nematics of planar initial orientation (induced by substrates covered with rubbed SE130 polyimide) were investigated in static electric fields by measurement of their optical transmittance influenced by planar deformation states. The splay and bend elastic constants and anchoring characteristics were determined from these experimental data. The polar anchoring for this nematics-substrate system can not be qualified uniquely as strong or weak. Simulated optical transmittance characteristics computed with using these parameters imitate results of experiment with good accuracy within measurement errors. It is demonstrated that precise determining of nematics-substrate coupling and nematics material parameters is sufficient for quantitative description of nematics deformations. Afterwards the values of components of the free energy of nematics layer corresponding to the bulk elastic deformation, bulk interaction with electric field, nematics interaction with boundary and splay-bend surface contribution are computed from experimental data in two cases which can be interpreted as weak and strong anchoring. The following comparison of them leads to conclusions on the negligible magnitude order of the splay-bend elastic constant.

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**Keywords:** anchoring of nematic molecules; nematic liquid crystals; nematics elastic constants; nematics-substrate coupling; polar anchoring characteristics; splay-bend nematics elastic constant

### INTRODUCTION

Stationary states of nematic liquid crystals are described by a unit dimensionless vector field with no defined sense, called director, that represents a locally averaged direction of nematic rode-like molecules. The corresponding governing equations can be derived as the Euler-Lagrange equations for a free energy functional defining the constitutive relationships for a nematics under study. The free energy functional of a nematics filling a volume V confined with a surface S, influenced by external electric and magnetic fields, can be considered in the form of a sum of bulk and surface functionals

$$F = \iiint\limits_V (f_K + f_E + f_M + f_A + f_D) dV + \oiint\limits_S f_S dS, \qquad (1a)$$

$$F = \iiint\limits_{V} (f_K + f_E + f_M) dV + \iint\limits_{S} (f_S + f_{AS} + f_{DS}) dS. \tag{1b}$$

The bulk free energy density consists of three terms: elastic distortion energy which has a commonly accepted basic form with the splay, twist and bend elastic constants:

$$f_K = \frac{1}{2} \left[ K_{11} (\nabla \cdot \mathbf{n})^2 + K_{22} (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33} (\mathbf{n} \times \nabla \times \mathbf{n})^2 \right]$$
 (2)

and energies of interactions of a nematics with electric or magnetic field

$$f_E = -\frac{1}{2} \mathbf{E} \cdot \mathbf{D}, \quad f_M = -\frac{1}{2} \mathbf{H} \cdot \mathbf{B}.$$
 (3)

Two questions that remain under discussion [1–11] are how to describe the boundary conditions by the free energy density of nematics-substrate interaction  $f_S$  and how to account the second-order terms with saddle-bend and splay-bend elastic constants  $K_{24}$  and  $K_{13}$ :

$$f_A = K_{13} \nabla \cdot [(\nabla \cdot \mathbf{n})\mathbf{n}], \tag{4}$$

$$f_D = -\frac{1}{2}(K_{22} + K_{24})\nabla \cdot [(\nabla \cdot \mathbf{n})\mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}]$$

$$= -\frac{1}{2}(K_{22} + K_{24})\nabla \cdot [(\nabla \cdot \mathbf{n})\mathbf{n} - (\mathbf{n} \cdot \nabla)\mathbf{n}]. \tag{5}$$

These two questions are commented in this work on the basis of the boundary conditions providing quantitative description of experimental results.

Under assumption of twice continuous differentiability of the director, two surface elasticity terms can be accounted in surface functional with corresponding surface densities:

$$f_{AS} = K_{13} \mathbf{k} \cdot [(\nabla \cdot \mathbf{n})\mathbf{n}] \tag{4'}$$

$$f_{DS} = -\frac{1}{2}(K_{22} + K_{24})\mathbf{k} \cdot [(\nabla \cdot \mathbf{n})\mathbf{n} - (\mathbf{n} \cdot \nabla)\mathbf{n}], \tag{5'}$$

with the unit vector field k of external normal on S; the confining surface S is assumed to be sufficiently smooth. These two terms, introduced by Frank [1] and Nehring and Saupe [2] have been extensively discussed recently [3–11]. The bulk free energy functional can be considered if form (1a) involving terms (4), (5) or in form (1b) involving terms (4'), (5').

The saddle-bend component (5) of the free energy density is rather apparently a second-order term, since it can be expressed with using only first-order derivatives of the director components (cf. [1,9,10,11]). Moreover it is a null Lagreangean [9,10] which does not contribute to bulk free energy and can be accounted in the form of a surface integral like in (1b). Concerning the elastic free energy functional with the density  $f_K + f_E + f_M$  as well as  $f_K + f_E + f_M + f_D$  leads to well-posed boundary-value problems for non-linear differential equations [9,10,11].

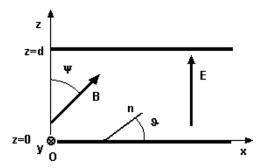
The splay-bend component (4) of the free energy density causes serious problem with minimisation of the functional (1a) or (1b) [3–11]. The functional becomes unbounded from below and the resulting boundary-value problem for the Euler-Lagrange equations is ill-posed [3,4,7–11]. Moreover, the second-order term (4) can not be transformed into the first-order one, contrary to the term (5). Although some theoretical remedies are discussed (cf. e.g. [3–8]), this problem is not definitively resolved.

Simultaneously, several theoretical proposals for characterising the nematics-substrate coupling, even in the case of basic configurations of planar or homeotropic nematics orientation, do not provide quantitative description of this phenomena. Particularly it is not clear whether the surface-like elasticity terms  $f_{AS}$  and  $f_{DS}$  can be included into the free boundary energy density  $f_S$  or should be considered separately [3–11].

The approach proposed in this work is based on the opinion that all second-order terms should be omitted from the free energy functional (1a) and the bulk elastic free energy density should be accounted in form of  $f_K$  (2); more arguments for such solution will be published elsewhere. Moreover, it is assumed and will be demonstrated that accounting only the boundary free energy density  $f_S$  in functional (1b) (without  $f_{AS}$  and  $f_{DS}$  terms) is enough to describing the nematics stationary states quantitatively when the anchoring characteristics are determined from experimental observations of nematic liquid crystal cells, at least for planar cells. Since only planar deformation states are considered, the discussion focuses on more problematic splay-bend surface elasticity term.

### PLANE STATIC DEFORMATIONS OF NEMATICS LAYER

A flat-parallel nematics cell is very well approximated as a flat layer, infinitely extended in two directions (Ox and Oy), with plane boundaries perpendicular to Oz axis, as sketched in Figure 1. The stationary states of such layer have the form of planar deformations if external field vectors (a magnetic field B with angle  $\psi$  to axis Oz or an electric field induced by a voltage U) and anchoring direction are all in the same plane (as in Fig. 1) and then (in one-dimensional approximation) can be fully characterised by the tilt angle  $\vartheta(z)$ . The total free energy



**FIGURE 1** Sketch of experimental configuration of a flat-parallel nematic cell in external fields. The director, Oz axis and external field vector are all in the same plane Oxz. The one-dimensional approximation is considered:  $\mathbf{n}(z) = (\cos \vartheta(z), 0, \sin \vartheta(z)), \mathbf{E}(z) = (0, 0, \mathbf{E}(z)), \mathbf{B}(z) = (B\sin \psi, 0, B\cos \psi).$ 

of a planar strain state per unit layer surface area may be then represented as

$$F = [F_K + F_E + F_M] + F_S + [F_{AS} + F_{DS}]$$

$$= \int_0^d f(\vartheta, \vartheta') dz + [f_1(\vartheta_1) + f_2(\vartheta_2)] + F_{AS}$$
(6)

(following from (1), (2), (3)) where  $f(\vartheta, \vartheta')$  – is the density of the bulk free energy of nematics elastic deformation and of the interactions of director field with external electric and magnetic fields,  $f = f_K + f_E + f_M$ ;  $F_S = f_1(\vartheta_1) + f_2(\vartheta_2)$  – is the boundary free energy in case of weak (finite) anchoring of nematic molecules at the layer boundaries;  $\vartheta_1 = \vartheta(0)$ ,  $\vartheta_2 = \vartheta(d)$ ,  $\vartheta'(z) = d\vartheta/dz$  (z). In general, taking the boundary free energy in the free energy functional (1b) can be alternatively substituted with taking suitable boundary conditions for the director field immediately, i.e., the nematics-substrate coupling characteristics (or anchoring characteristics) can be accounted in the form of a functional with a density  $f_S$  or in the form of boundary conditions. In case of strong anchoring the last variant is more convenient. In this nematics cell configuration  $f_{DS} = 0$  and  $F_{AS} = -K_{13} \sin(\vartheta_1) \cos(\vartheta_1) \vartheta'(0) + K_{13} \sin(\vartheta_2) \cos(\vartheta_2) \vartheta'(d)$ .

Symmetric boundary conditions when  $f_S = f_1 = f_2$  depends only on  $\vartheta(0) = \vartheta(d)$  and not on  $\vartheta'(0)$  will be considered here. Moreover, firstly functional (6) will be analysed with  $K_{13} = 0$  and  $F_{AS} = 0$ . A function  $\vartheta = \vartheta(z)$  minimising functional (6) with  $F_{AS} = 0$  must satisfy the Euler-Lagrange equations for it:

$$\frac{\partial f}{\partial \theta} - \frac{d}{dz} \frac{\partial f}{\partial \theta'} = 0 \qquad \text{for } 0 < z < d 
- \left(\frac{\partial f}{\partial \theta'}\right)_{|z=0} + \frac{df_1}{d\theta_1} = 0 \quad \text{for } z = 0 
\left(\frac{\partial f}{\partial \theta'}\right)_{|z=d} + \frac{df_2}{d\theta_2} = 0 \quad \text{for } z = d$$
(7)

The two last equations can be interpreted as the balance of a torque per cell unit surface area induced by a nematics-substrate interaction, e.g.  $\tau_1(\vartheta(0)) = df_1/d\vartheta_1(\vartheta(0))$ , with a torque from the deformed bulk,  $(\partial f/\partial\vartheta')(\vartheta(0),\vartheta'(0))$ , induced by external fields, that can be calculated with using the first equation:  $T_b = \tau(\vartheta(0)) = \tau(\vartheta(d)) = (\partial f/\partial\vartheta')(\vartheta(d),\vartheta'(d)) = \int_0^d \partial f/\partial\vartheta(\vartheta(z),\vartheta'(z))dz$ . Hence these two equations can be interpreted as boundary conditions of the form  $\vartheta(0) = \vartheta(d) = \Theta(T_b)$  with a function  $\Theta$  (inverse to  $\tau$ ,  $\Theta = \tau^{-1}$ ) describing the nematics-substrate coupling. The tilt angle  $\vartheta(z)$  should then satisfy the following

equations (cf. e.g. [13]):

$$(K_{11}\cos^{2}\vartheta + K_{33}\sin^{2}\vartheta)\vartheta'' + (K_{33} - K_{11})\sin\vartheta\cos\vartheta \cdot \vartheta'^{2} + \frac{\varepsilon_{0}\varepsilon_{a}\varepsilon_{e}^{2}U^{2}\sin\vartheta\cos\vartheta}{d^{2}(\varepsilon_{\perp}\cos^{2}\vartheta + \varepsilon_{\parallel}\sin^{2}\vartheta)^{2}} + \frac{\chi_{a}B^{2}}{\mu_{0}}\sin(\vartheta + \psi)\cos(\vartheta + \psi) = 0$$

$$\varepsilon_{e} = \left\{\frac{1}{d}\int_{0}^{d}\frac{1}{\varepsilon_{\perp}\cos^{2}\vartheta(z) + \varepsilon_{\parallel}\sin^{2}\vartheta(z)}dz\right\}^{-1}$$
(8)

where  $\varepsilon_a = \varepsilon_{||} - \varepsilon_{\perp}$  is the anisotropy of electric permittivity,  $\chi_a = \chi_{||} - \chi_{\perp}$  is the anisotropy of diamagnetic susceptibility,  $\varepsilon_e$  is the effective electric permittivity of the nematics layer, and boundary conditions [12,13]:

$$T_{b} = \int_{0}^{d} \left[ (K_{11} - K_{33}) \sin \vartheta(z) \cos \vartheta(z) \vartheta'(z)^{2} \right] dz$$

$$+ \int_{0}^{d} \left[ \frac{\varepsilon_{0} \varepsilon_{a} \varepsilon_{e}^{2} U^{2} \sin \vartheta(z) \cos \vartheta(z)}{d^{2} \left[ \varepsilon_{\perp} \cos^{2} \vartheta(z) + \varepsilon_{||} \sin^{2} \vartheta(z) \right]^{2}} \right.$$

$$+ \frac{\chi_{a} B^{2}}{\mu_{0}} \sin(\vartheta(z) + \psi) \cos(\vartheta(z) + \psi) \right] dz,$$

$$\vartheta(0) = \vartheta(d) = \Theta(T_{b}). \tag{9}$$

The boundary function  $\Theta(T_b)$  should be non-decreasing for positive values of  $T_b$ ; in this work it is modelled by a non-decreasing cubic spline.

## DETERMINATION OF NEMATICS PARAMETERS BY SOLVING INVERSE PROBLEM

The director field inside a nematic liquid crystal cell can hardly be determined in immediate experiment. The observed physical quantity is usually some functional dependent on cell deformation state, like flat cell electric capacitance or optical transmittance or optical retardation. In this work the optical retardation of a cell as birefringent system is used as this monitoring physical quantity.

A dependence of the phase shift  $\varphi = \varphi(U; B, \psi)$  between ordinary and extraordinary rays of light transmitted through a flat cell on nematics deformation (optical retardation),

$$\varphi = \frac{2\pi}{\lambda} d \left[ \frac{1}{d} \int_0^d \frac{n_e \cdot n_o}{\sqrt{n_e^2 \cdot \sin^2 \vartheta(z) + n_o^2 \cdot \cos^2 \vartheta(z)}} dz - n_o \right], \quad (10)$$

where  $n_o$  and  $n_e$  are ordinary and extraordinary refractive indices, being influenced by external fields, contains the information about material constants, e.g.  $K_{11}$ ,  $K_{33}$ ,  $\chi_a$ ,  $\Theta$  (where  $\Theta$  states now for spline coefficients).

Let  $p=(K_{11},\ K_{33},\ \chi_a,\ \Theta)$  denote the set of unknown material parameters. For any sequence of k measurements  $(\varphi_e(U^i;B^i,\psi^i))_{i=1}^k$  one can calculate a corresponding sequence of values of light phase shift  $(\varphi_c(U^i;B^i,\psi^i;p))_{i=1}^k$  using formulae (8), (9), (10). The sought magnitudes of material parameters p can be determined as corresponding to the minimal value of the objective functional (or the similarity functional):

$$S(p) = \left\{ \frac{1}{k} \sum_{i=1}^{k} \left[ \frac{\varphi_e(U^i; B^i, \psi^i) - \varphi_c(U^i; B^i, \psi^i; p)}{\varphi_e(U^i; B^i, \psi^i)} \right]^2 \right\}^{\frac{1}{2}}, \tag{11}$$

being the discrepancy between the sets of experimental and simulated values of monitoring quantity. The minimisation of (11) with finding magnitudes of material constants is realised with the use of immediate methods of optimisation [12,13].

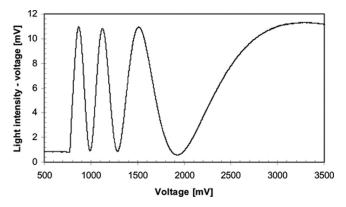
A set p of nematics parameters to be determined can be extended with other material constants like  $K_{22}$  (for problems with twisted nematics) or  $\varepsilon_{||}$  and  $\varepsilon_{\perp}$  or  $n_o$  and  $n_e$  (that can be measured immediately, as in this work).

#### EXPERIMENT AND COMPUTATIONS

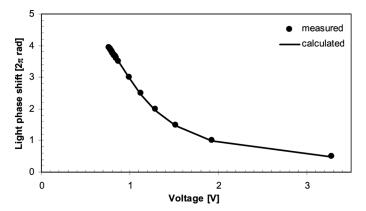
One wedge nematic cell and three flat cells were made of glass plates (of size  $22 \times 35\,\mathrm{mm}$ ), coated with indium-tin oxide electrodes and orienting layer of rubbed polyimide SE130, and were filled with 4'-pentyl-4-cyanobiphenyl (5CB). The plates for the wedge cell were glued without a spacer along one edge and with a spacer (of thickness about  $200\,\mu\mathrm{m}$ ) along the other. The orientation of nematics molecules enforced by rubbed substrates was parallel to the boundaries and to the wedge edge in the wedge cell or parallel to the boundaries and each other at both substrates in flat cells. Each cell was investigated in a thermostatic stage between a polariser and analyser crossed in the measurement system, consisting of a He-Ne laser and a microscope with a photodetector. In the wedge cell a system of interference fringes from a normally incident light appeared (in the absence of external fields):  $\Phi_j = 2\pi j$ ,  $d_j = j\lambda n_a^{-1}$ ,  $n_a \equiv n_e - n_0$ , where j is the order of

the interference minimum,  $d_j$  is the corresponding cell thickness,  $\Phi_j$  is the phase shift and  $\lambda$  is the light wavelength. In the small neighbourhood of each fringe position a wedge cell can be treated as the planar one (like sketched in Fig. 1) due to very small wedge angle (about 10 mrad).

The intensity of normally incident light transmitted through the cell birefringence system in the positions of selected interference fringes as a function of voltage (sine-wave with frequency of 1.5 kHz) was recorded for 2th to 9th fringes in the wedge cell (corresponding to the cell thickness  $6.9 \,\mu\text{m} \div 31.2 \,\mu\text{m}$ ) and for the three flat cells of thickness  $1.9 \,\mu\text{m}$ ,  $3.3 \,\mu\text{m}$  and  $5.3 \,\mu\text{m}$ , at temperature of  $22.6 \,^{\circ}\text{C}$ . In such experiment a wedge cell was equivalent to a system of planar cells of different thicknesses. The temperature was stabilised with accuracy within 0.1°C. The driving voltage was changed during measurements so slowly that all deformation states could be considered as static caused by static external fields (of magnitude equal to effective voltage). After determining the optical retardation from electric transmission characteristics (as illustrated in Figs. 2, 3 and 4), the sets of pairs  $(U, \varphi)$  were input data for extracting the sought values of material parameters as solutions to the corresponding inverse problems. The inverse problem was solved for each cell separately by approximate finding the minimum of the objective functional (11) and corresponding magnitudes of splay and bend elastic constants,  $K_{11}$  and  $K_{33}$ , together with a nematics-substrate coupling characteristic  $\Theta = \Theta(T_h)$  (in the form of non-decreasing cubic spline). Afterwards,

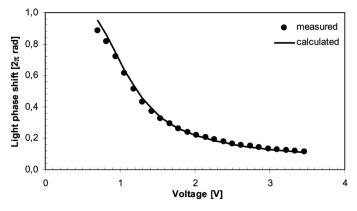


**FIGURE 2** Intensity of normally incident light (expressed as equivalent voltage), transmitted through the wedge cell in the place of appearing fourth interference fringe, corresponding to the cell thickness of  $13.9\,\mu m$ , as a function of voltage, measured at temperature of  $22.6^{\circ}C$ .

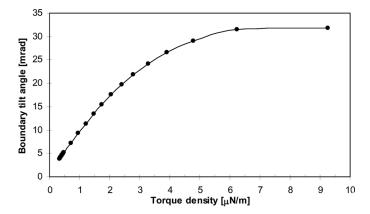


**FIGURE 3** Optical retardation corresponding to selected points (including subsequent extreme points) of the curve in Figure 3 as a function of applied voltage — measured and calculated with the refined material parameters; the resulting value of the objective functional is  $S(p) \approx 0.011$ .

the average solution was chosen to achieve the optimal-like approximation for all analysed cells with same material parameters. The other nematics parameters were measured previously:  $\varepsilon_{||}=19.04$ ,  $\varepsilon_{\perp}=6.50$ ,  $n_o=1.5383$  and  $n_e=1.7206$  (at temperature of  $22.6^{\circ}C$ ). In this way,  $K_{11}=6.7pN$ ,  $K_{33}=8.5pN$  and the dependence of the boundary tilt angle on the torque density displayed in Figure 5 were obtained as the solution to the inverse problem. Then the values of



**FIGURE 4** Optical retardation (corresponding to selected points of the transmission curve) as a function of applied voltage – measured and calculated with the refined material parameters for the flat cell of thickness of  $3.3\,\mu m$ ; the resulting value of the objective functional is  $S(p)\approx 0.035$ .



**FIGURE 5** Director boundary value as a function  $\vartheta(0)=\vartheta(d)=\Theta(T_b)$  of the torque per cell unit surface area (transmitted to the boundary from the bulk) describing approximately the coupling between the 5CB nematics and the substrate made of the rubbed SE130 polyimide. The anchoring is strong for large magnitudes (with  $\vartheta(0)=\vartheta(d)=\vartheta_{0s}\approx 31.8$  mrad) of the torque density and weak for small ones. It may not be clearly qualified as weak or strong. In computations it is convenient to use this function, describing the dependence of the boundary values of the tilt angle on the torque density, instead of the inverse one (Fig. 6). By approximating  $\Theta(T_b)\approx \Theta_0+\Theta_1T_b$  (for smaller  $\vartheta(0)$ ) one obtains the anchoring angle  $\vartheta_0=\Theta_0\approx 0.5$  mrad and the polar anchoring energy coefficient  $W=\Theta_1^{-1}\approx 101\mu Jm^{-2}$ .

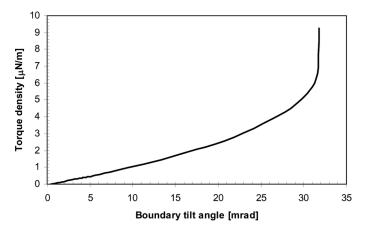
the optical retardation dependent on voltage applied to the cell were computed for each cell with using these parameters, and compared with the measured ones; examples are displayed in Figures 3 and 4. The resulting values of the objective functional are collected in Table 1. They accord well with estimates of measurement errors. The anchoring angle  $\theta_0 = \Theta_0$  and the polar anchoring energy coefficient  $W = \Theta_1^{-1}$  can be estimated by approximating  $\Theta(T_b) \approx \Theta_0 + \Theta_1 T_b$  (for smaller  $\theta(0)$ ); that corresponds to an approximation  $f_S(\theta(0)) \approx 1/2W(\theta(0) - \theta_0)^2$ 

A possible significance of a free splay-bend surface elastic energy term was studied via determining components of the free energy per cell unit surface area from experimental data. These components as a

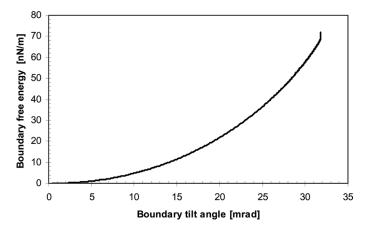
**TABLE 1** Discrepancies Between the Simulated and Measured Optical Retardation

$d[\mu m]$	1.9	3.3	5.3	6.9	10.4	13.9	17.3	20.8	24.3	27.8	31.2
S(p)	0.067	0.035	0.042	0.025	0.016	0.011	0.009	0.012	0.010	0.013	0.019

function of effective voltage applied to cell covers were calculated for two model examples: a case of weak anchoring in the equivalent flat cell of thickness of 13.9 µm in the place of appearing fourth interference fringe in the wedge cell (when an electric field induced by a voltage was so weak, that under a torque from a deformed nematics bulk the boundary tilt angle was less than the saturation level,  $\vartheta(0) = \vartheta(d) < \vartheta_{0s} \approx 31.8 \,\mathrm{mrad}$ , cf. Fig. 5) and a case of strong anchoring in the flat cell of thickness of 3.3 µm (when an electric field was so strong, that the boundary tilt angle attained the saturation level of  $\vartheta(0) = \vartheta(d) = \vartheta_{0s}$ ). For each selected voltage, having a tilt angle  $\vartheta(z)$ ,  $0 \le z \le d$  (i.e., a director field) determined as a part of a solution to the inverse problem, one calculated a bulk free energy of nematics elastic deformation and of the interactions of director field with external electric field, a boundary free energy of the interaction of a nematics with layer boundaries (only in case of weak anchoring) and a free surface elastic energy (only the splay-bend term with  $K_{13} = 6$ pN). The hypothetical value of  $K_{13} = 6$ pN close to  $K_{11} = 6.7$ pN and  $K_{33} = 8.5 \,\mathrm{pN}$  was assumed to compare the magnitudes of corresponding free energy components. In the considered nematics cell configuration  $F_{DS} = 0$ ,  $F_S = f_S(\vartheta(0)) + f_S(\vartheta(d))$  (Fig. 7) was found by numerical integration of the inverse boundary function  $\Theta^{-1}(T_b) =$  $\tau(\vartheta(0)) = df_S/d\vartheta(0)(\vartheta(0))$  (Fig. 6),  $F_{AS}$  was calculated from boundary values of the tilt angle and its derivative:



**FIGURE 6** Torque per cell unit surface area  $[\mu Jm^{-2}]$  as a function of the director boundary value  $T_b = \Theta^{-1}(\vartheta(0)) = \Theta^{-1}(\vartheta(d))$  [mrad] describing approximately the coupling between the 5CB nematics and the substrate made of the rubbed SE130 polyimide; for  $\vartheta(0) = \vartheta(d) < \vartheta_{0s}$  it is the inverse function to  $\vartheta(0) = \Theta(T_b)$  displayed in Figure 5.

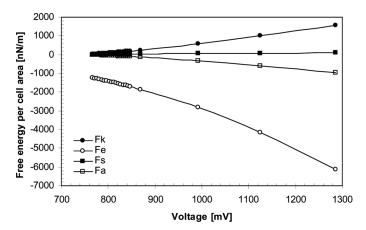


**FIGURE 7** Boundary free energy of the interaction between the 5CB nematics and the substrate made of the rubbed SE130 polyimide (per cell unit surface area [nJm<sup>-2</sup>]) as a function of the director boundary value  $\vartheta(0) = \vartheta(d)$  [mrad] obtained by numerical integration of function  $T_b = \Theta^{-1}(\vartheta(0)) = \Theta^{-1}(\vartheta(d))$  displayed in Figure 6.

 $F_{AS} = -K_{13}\sin(\vartheta(0))\cos(\vartheta(0))\vartheta'(0) + K_{13}\sin(\vartheta(d))\cos(\vartheta(d))\vartheta'(d), \quad F_{M} = 0$  (since B = 0),  $F_{K}$  and  $F_{E}$  were calculated via numerical integration:

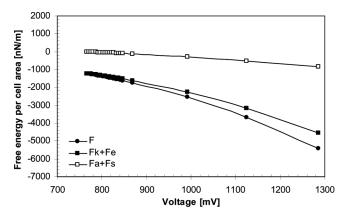
$$\begin{split} F_K &= \frac{1}{2} \int_0^d \left( K_{11} \cos^2 \vartheta(z) + K_{33} \sin^2 \vartheta(z) \right) [\vartheta'(z)]^2 dz, \\ F_E &= -\frac{\varepsilon_0 U^2}{2d} \left\{ \frac{1}{d} \int_0^d \frac{1}{\varepsilon_\perp \cos^2 \vartheta(z) + \varepsilon_\parallel \sin^2 \vartheta(z)} \, dz \right\}^{-1}. \end{split}$$

The relations of free energy components are quite different in two cases. In both cases  $F_K$ ,  $F_S > 0$  and  $F_E$ ,  $F_{AS} < 0$ . In case of weak anchoring (Figs. 8 and 9)  $F_E$  dominates and roughly  $F_K < \frac{1}{4}|F_E|$ ,  $|F_{AS} + F_S| < \frac{1}{8}|F_K + F_E|$ ,  $|F_S| \approx \frac{1}{40}|F_K + F_E|$ ,  $|F_S| \approx \frac{1}{8}|F_{AS}|$ . In case of strong anchoring (Figs. 10 and 11)  $|F_K|$  dominates and roughly  $|F_E| < \frac{1}{2}F_K$ ,  $|F_{AS}| < \frac{1}{15}|F_K + F_E|$ ,  $|F_{AS}| \approx \frac{1}{30}F_K$  and a reliable estimate of  $|F_S|$  is impossible due to measurements errors (instead of assuming  $|F_S| = \infty$  other components of free energy are considered with restriction for boundary condition  $|\Im(0)| = \Im(d) = \Im_{0s} \approx 31.8 \, \mathrm{mrad}$ ). In both cases if  $|F_{AS}| = 0$  were of assumed order (with  $|F_S| = 0$ ), it would influence a total free energy significantly, in case of weak anchoring additionally  $|F_{AS}| = 0$  dominated  $|F_S| = 0$ . A precise characterisation of nematics-substrate coupling (like displayed in Fig. 5) enables quantitative description of

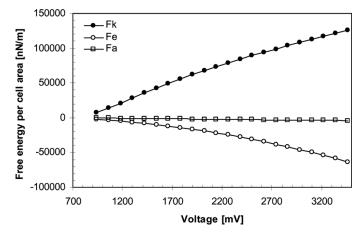


**FIGURE 8** Free energies per cell unit surface area  $[nJm^{-2}]$  as functions of effective voltage, calculated for the equivalent flat cell of thickness of  $13.9\,\mu m$  in the place of appearing fourth interference fringe in the wedge cell, in case of weak anchoring of the 5CB nematics and the substrate made of rubbed SE130 polyimide.

analysed phenomena (as illustrated in Table 1 and Figs. 3 and 4). The obtained results then can be interpreted in two ways: accounting term  $F_{AS}$  is not necessary for an adequate description of phenomena or

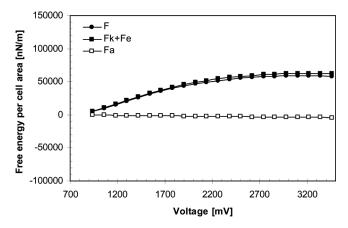


**FIGURE 9** Total, bulk and surface free energies per cell unit surface area  $[nJm^{-2}]$  as functions of effective voltage (obtained by adding components displayed in Fig. 8), calculated for the equivalent flat cell of thickness of  $13.9\,\mu m$  in the place of appearing fourth interference fringe in the wedge cell, in case of weak anchoring of the 5CB nematics and the substrate made of rubbed SE130 polyimide.



**FIGURE 10** Free energies per cell unit surface area  $[nJm^{-2}]$  as functions of effective voltage, calculated for the flat cell of thickness of  $3.3\,\mu m$ , in case of strong anchoring of the 5CB nematics and the substrate made of rubbed SE130 polyimide.

neglecting term  $F_{AS}$  should interfere the adequacy of this description. It leads to the conclusion that this term can be omitted from free energy functional or, alternatively, that  $K_{13} \approx 0$ .



**FIGURE 11** Total, bulk and surface free energies per cell unit surface area [nJm<sup>-2</sup>] as functions of effective voltage (obtained by adding components displayed in Fig. 10), calculated for the flat cell of thickness of 3.3 μm, in case of strong anchoring of the 5CB nematics and the substrate made of rubbed SE130 polyimide.

### CONCLUSIONS

Accurate determination of the boundary condition (i.e., the anchoring characteristics), together with the elastic constants, like presented here, enables to describing planar deformation states of a nematics layer quantitatively and precisely. The boundary free energy functional depending only on the boundary values of the tilt angle and not on its derivative is sufficient for characterising nematicssubstrates interaction adequately. The simulation of the optical retardation, with using the same magnitudes of splay and bend elastic constants and anchoring characteristics, for flat nematics cells with thickness from  $1.9 \,\mu m$  to  $31.2 \,\mu m$ , results in reproducing the measured values with the accuracy inferior to experimental errors. It implies that there is no dependence of the bulk elastic constants on the nematics cell thickness and that there is no need to exploit surface-like elastic constants (and corresponding free elastic energy terms) for the description of nematics as material continuums. A similar conclusion was drawn previously from experiments with cells of thickness from  $13.9\,\mu m$  to  $64.5\,\mu m$  [12]. Although only planar deformation states enforced in planar cells by static electric field were investigated, this conclusion seems to be valid in another cases.

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