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Microscopic and macroscopic description of anchoring at the nematic-solid substrate interface

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A simple microscopic mean-field model for a flat nematic liquid crystal (NLC) sample in a contact to the solid substrate surface is offered. An interaction between NLC molecules is simulated by the well known McMillan model potential, and an orienting action of the solid substrate surface on NLC molecules is modeled by a short-range external field which acts directly only on molecules within the first molecular layer of the nematic sample adjacent to the substrate surface. For an undistorted NLC sample, the model allows the calculation of local order parameter profiles for different values of strength of this external orienting field and temperature of the sample. These profiles are used in a description of a director field distortion caused by a certain external action and in the calculation of the anchoring energy coefficient W used in a macroscopic description of the anchoring at the nematic-solid substrate interface. Dependence of this coefficient on the strength of the short-range orienting field is obtained, and an unequivocal relation between the magnitude of W and the orientational order parameter profile near the substrate surface is established. The temperature dependence of the coefficient W calculated from the offered microscopic model is in good agreement with the experimental data on NLC MBBA.

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I. INTRODUCTION

The interactions between liquid crystal (LC) molecules and a solid substrate surface are of both fundamental and technological interest [1,2]. From all liquid crystalline phases, the nematic LC (NLC) phase is most sensitive to these interactions. The NLC-solid substrate surface interactions change the structure and properties of the nematic interfacial layer. The orientational order in this interfacial layer, and, hence, its electro-optic and viscoelastic properties, can be significantly different from analogous characteristics of NLC bulk [3–11], and smectic layering structures [12–16], which does not occur in the bulk nematic phase, can also appear near the solid substrate surface. In addition, the NLC-solid substrate surface interactions define boundary conditions for the whole macroscopic NLC sample, and, depending on a treatment of this surface, these interactions impose various types (homeotropic, planar, tilt) of alignment on the nematic sample [1,2,17–24]. This alignment determines completely the behavior of the NLC sample under applied external fields, an optical uniformity of flat NLC layers used in various displays and optical valves, threshold fields, and operating times of these devices [25–27].

In the framework of the continuous theory of the elastic NLC deformations, an orienting action of the solid substrate surface on a NLC sample, or so-called the NLC-substrate anchoring [1,2], is described by means of two fundamental notions, namely, the easy axis of alignment $\vec{\gamma}$, and the anisotropic contribution f_s to the interfacial free energy of NLC. In the absence of external fields, the director $\vec{n}$, which defines a preferred average orientation of the LC molecules [28,29], is parallel to $\vec{\gamma}$, and this alignment of $\vec{n}$ minimizes the anisotropic contribution f_s to the interfacial free energy of NLC. If our NLC sample is under the action of a certain external field (electric, magnetic, or field of deformations induced by another boundary surface of the sample), the director $\vec{n}$ deviates from the easy axis of alignment $\vec{\gamma}$, and this deviation is associated with an increase $\Delta f_s(\theta_s)$ in the anisotropic contribution to the interfacial free energy of the sample. Here, θ_s is the polar angle formed by the director $\vec{n}$ and the easy axis of alignment $\vec{\gamma}$ just at the solid substrate surface. The simplest and most frequently used in practical calculations expression for $\Delta f_s(\theta_s)$ can be written as [30]

$$\Delta f_s(\theta_s) = \frac{1}{2} W \sin^2 \theta_s, \qquad (1)$$

or, in the case of small angle θ_s,

$$\Delta f_s(\theta_s) \approx \frac{1}{2} W \theta_s^2. \qquad (2)$$

The experimental and theoretical determination of the coefficient W in Eqs. (1) and (2), which is called the anchoring strength or anchoring energy coefficient (in real experiments, the anchoring extrapolation length $L_0 = K/W$ [1,2], where K is one of NLC elastic constants, is measured), is one of the most important topics in the physics of LCs.

A value of the coefficient W, as well as the direction of the easy axis of alignment $\vec{\gamma}$, depends on the type of surfactant deposited on the solid substrate surface, on a treatment of this surface (mechanical rubbing, SiO films evaporation under oblique incidence, etching, annealing, etc.), and on the type of LC contacting to the substrate surface [2,18,19]. Usually, this value ranges from $\sim 10^{-3}$ erg/cm^2 (10^{-6} J/m^2) ("weak" anchoring) up to $\sim$erg/cm^2 (10^{-3} J/m^2) ("strong" anchoring). It is obvious that the phenomenological coefficient W is determined by the direct interaction between LC molecules and the substrate surface [31], and one could find a certain relation connecting the magnitude of W to the strength of this interaction and, hence, to the microscopic structure of the interfacial LC layer, and there is a number of

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*Email address: miran@microm.ipme.ru; miran@mail.ru theoretical papers [32–38] devoted to the determination of this relation. Up to now, however, this problem is very far from its complete solution.

In the present paper we offer a simple microscopic mean-field model for a flat NLC sample in a contact to the solid substrate surface (similar model for description of behavior of free-standing LC films upon their heating was proposed in our previous papers [39,40]). The NLC sample is assumed to be composed of N flat layers parallel to the substrate surface and having a thickness of the order of the molecular length l_0. An interaction between LC molecules is modeled by a well known anisotropic McMillan's pair potential [41], and an orienting action of the substrate surface on NLC is simulated by a short-range external field which acts directly only on molecules within the first molecular layer of the sample. When the NLC sample is undistorted (local directors for all layers of the sample coincides with the easy axis of alignment imposed by the substrate), in the framework of a mean-field approximation, expressions for one-particle pseudopotentials for molecules of each layer of the sample are derived, and the local orientational order parameters, which characterize the orientational order within each molecular layer, are determined. Self-consistent equations for these local order parameters are also derived, and expressions for both the free energy of each molecular layer and the total free energy of the sample are obtained. Numerical solution of these self-consistent equations gives the local orientational order parameter profiles as a function of both the strength of direct interaction between NLC molecules and the substrate surface and the temperature of the sample. Then, we consider a deformation of the sample induced by a certain external action (the local director of the last Nth layer of the sample is assumed to be rotated by the angle $\theta_N = \pi/2$ with respect to an initial direction of an equilibrium alignment of the sample which is assumed, for a certainty, to be homeotropic). An excess free energy ΔF associated with this deformation is determined as a function of angles θ_i, which determine deviation of the local directors $\vec{n}_i$ from their initial equilibrium alignment. Minimizing ΔF with respect to θ_i, one can obtain a set of equations which determine a profile of angles θ_i in whole NLC sample including its interfacial region. The extrapolation length L_0 is obtained from this profile, and, knowing a magnitude of the elastic constant K (if an initial alignment of the sample is homeotropic, K is equal to the bend elastic constant K_{33}), from the above-mentioned relation between L_0, K, and W, one can obtain the value of the anchoring energy coefficient W. Thus, we have obtained the dependence of this coefficient on the strength of the short-range anisotropic field acting on NLC molecules within the first molecular layer of the sample (as said above, in framework of the microscopic model offered here, this field simulates the direct orienting action of the substrate surface on the NLC sample). It has been found that the condition of "strong" anchoring must not necessarily correspond to the strength of this orienting action exceeding or even equal to that of the intermolecular interaction in NLC. For example, the ratio $W_0/V_0 \approx 0.1$, where W_0 is an interaction constant determining the strength of the above mentioned short-range orienting field and V_0 is an interaction constant of the intermolecular forces in NLC, corresponds to the anchoring energy coefficient $W \sim \mathrm{erg/cm^2}$ (10^{-3} J/m^2), or to the case of strong anchoring, whereas the coefficient $W \sim 10^{-2}$ erg/cm^2 (10^{-5} J/m^2) ("weak" anchoring) corresponds to $W_0/V_0 \sim 0.01$. It has also been found a simple and unequivocal relation between the orientational order parameter profile near the substrate surface and the magnitude of the coefficient W. When the orientational order parameter at the substrate surface is significantly larger than that in the NLC bulk, the "rigid" NLC-substrate anchoring occurs, i.e., any elastic deformation of the director field cannot penetrate into the first molecular layer of the NLC sample. When the orientational order parameter at the substrate surface is comparable to that in the NLC bulk, we deal to the case of the strong anchoring ($W \sim \mathrm{erg/cm^2}$). Finally, when the orientational order parameter at the substrate surface is significantly smaller than that in the NLC bulk, the weak anchoring ($W \sim 10^{-2}$ erg/cm^2) occurs. We have also investigated the temperature dependence of the anchoring extrapolation length L_0 for both weak and strong anchoring. It has been found that, for weak anchoring, the extrapolation length L_0 decays significantly with decreasing temperature, whereas, in the case of the strong anchoring, the extrapolation length is nearly temperature independent. The results of the numerical calculation of the anchoring energy coefficient W for NLC MBBA are in a good agreement with the experimental data.

We start in the next section with a description of the offered microscopic mean-field model for the undistorted flat NLC sample in a contact to the solid substrate surface. Then, we derive expressions for excess free energy of the sample associated with the director field distortion caused by a certain external action. Minimizing this excess free energy, we also obtain a set of equations which determine the profile of this distortion. Section III presents the results of the numerical calculations based on the results obtained in Sec. II and in the discussion.

II. MICROSCOPIC MODEL FOR A FLAT NLC SAMPLE IN A CONTACT TO THE SOLID SUBSTRATE SURFACE

A. Undistorted sample

Let us consider a flat NLC sample composed of N discrete layers having a thickness of the order of the molecular length l_0. The first molecular layer of the sample is in a contact to the solid substrate surface, and the last Nth layer has properties similar to those of the bulk NLC sample at the given temperature. The sample is assumed to be undistorted and homeotropically oriented, i.e., the local director $\vec{n}_i$ for each of its layers is aligned parallel to the normal $\vec{\nu}$ to the substrate surface. As in Refs. [39,40], we model an anisotropic intermolecular interaction in our sample by the well known McMillan's model pairwise potential [41]

$$V_{12}(r_{12},\vartheta_{12}) = -(V_0/n_0 r_0^3 \pi^{3/2})\left(\tfrac{3}{2}\cos^2\vartheta_{12} - \tfrac{1}{2}\right)\exp(-r_{12}^2/r_0^2), \tag{3}$$

where V_0 is the interaction constant, ϑ_{12} is the polar angle formed by long axes of interacting molecules, r_{12} is the distance between their centers, r_0 is the characteristic interaction length, and n_0 is the number of molecules per unit volume. Since, in the framework of the McMillan's theory, the length r_0 is assumed to be much smaller than the molecular length l_0; this interaction should almost completely decay at a distance of the order of the molecular length l_0, and one can assume that molecules within each molecular layer of the NLC sample interact only with molecules of the same layer and those of two neighboring layers. As in Refs. [39,40], an anisotropic interaction between NLC molecules and the substrate surface is assumed to be short-range and modeled by a certain orienting short-range field which acts directly only on molecules within the first molecular layer of the sample adjoining to the substrate surface. An energy of this interaction can be written as [39,40]

$$W_1(\vartheta_1) = -W_0\left(\tfrac{3}{2}\cos^2\vartheta_1 - \tfrac{1}{2}\right), \tag{4}$$

where ϑ_1 is the polar angle formed by the long axes of molecules within the first layer of the sample and the normal $\vec{\nu}$ to the substrate surface, and W_0 is the interaction constant determining the strength of this orienting field. By analogy with McMillan's theory [41], and taking into account the above-mentioned assumptions, in a mean-field approximation, from the potentials (3) and (4) one can derive one-particle pseudopotentials $V_i(\vartheta_i)$ [39,40] for molecules localized within each ith molecular layer of the sample. Here, ϑ_i is the polar angle formed by the long axes of molecules within the ith layer and the local director $\vec{n}_i$. Assuming that no translational smectic ordering occurs in the NLC sample under consideration, one can obtain

$$V_1(\vartheta_1) = -\tfrac{1}{3}V_0\left(\tfrac{3}{2}\cos^2\vartheta_1 - \tfrac{1}{2}\right)(s_1 + s_2 + 3W_0/V_0), \tag{5}$$

$$V_{2\le i\le N}(\vartheta_i) = -\frac{1}{3}V_0\left(\frac{3}{2}\cos^2\vartheta_i - \frac{1}{2}\right)\sum_{j=i-1}^{i+1} s_j, \tag{6}$$

where s_i are the local orientational order parameters for layers of the sample which are determined by the following self-consistent equations:

$$\begin{aligned} s_i &= \left\langle\left(\frac{3}{2}\cos^2\vartheta_i - \frac{1}{2}\right)\right\rangle \\ &= \int_{-1}^{+1}\left(\frac{3}{2}\cos^2\vartheta_i - \frac{1}{2}\right) f_i(\vartheta_i)\, d\cos\vartheta_i \\ &\quad \times\left(\int_{-1}^{+1} f_i(\vartheta_i)\, d\cos\vartheta_i\right)^{-1}. \end{aligned} \tag{7}$$

Here, $f_i(\vartheta_i)$ is the one-particle distribution function for molecules of the ith layer which is determined as

$$f_i(\vartheta_i) = A_i^{-1}\exp[-V_i(\vartheta_i)/K_BT], \tag{8}$$

where A_i is the normalizing constant for the ith layer, T is the absolute temperature of the sample, and K_B is the Boltzmann constant. The free energies F_i of the discrete molecular layers of the NLC sample are given by the following equations:

$$\begin{aligned} F_1 = N_iV_0\Bigg[&\frac{1}{6}s_1(s_1 + s_2) - \frac{K_BT}{V_0} \\ &\times\ln\left(\int_0^1 \exp[-V_1(\vartheta_1)/K_BT]\, d\cos\vartheta_1\right)\Bigg], \end{aligned} \tag{9}$$

$$\begin{aligned} F_{2\le i\le N} = N_iV_0\Bigg[&\frac{1}{6}s_i\sum_{j=i-1}^{i+1} s_j - \frac{K_BT}{V_0}\ln \\ &\times\left(\int_0^1 \exp[-V_i(\vartheta_i)/K_BT]\, d\cos\vartheta_i\right)\Bigg], \end{aligned} \tag{10}$$

where N_i is a number of molecules within a single molecular layer. The total free energy F of the sample is given by

$$F = \sum_{i=1}^{N} F_i. \tag{11}$$

Since, far from the substrate surface, the NLC sample under consideration is spatially uniform, in Eqs. (6) and (10), the local order parameter s_{N+1} for the $N+1$ layer should be set equal to that for the Nth layer, i.e., s_N. The numerical solution of self-consistent equations (7) allows one to determine the local orientational order parameters s_i for a given number N of layers of the NLC sample, the reduced temperature $T^* = K_BT/V_0$, and the ratio W_0/V_0, and Eqs. (9)–(11) enable us to calculate, from these values of the order parameters s_i, the free energy F_i for each molecular layer of the sample and its total free energy F.

B. Microscopic description of distortion in the NLC sample

Now, let us consider a distortion in the NLC sample in a contact to the solid substrate surface. The distortion can be induced by either external fields or another substrate surface inducing an orientation different from the homeotropic alignment induced by the first substrate, for example, planar. Not concretizing a way of imposing this distortion on the sample, let us assume that the local director $\vec{n}_N$ of its last Nth layer forms the angle $\theta_N = \pi/2$ with respect to its initial alignment. As a result, the local director $\vec{n}_i$ of each ith layer deviates from its initial alignment $\vec{\nu}$ by the angle θ_i, and it forms the angles $\theta_{i,i-1}$ and $\theta_{i,i+1}$ with the local directors $\vec{n}_{i-1}$ and $\vec{n}_{i+1}$, respectively, of its two neighboring layers. If the substrate is assumed to be perfectly flat, and the NLC sample under consideration is sufficiently thick ($N \gg 1$), profiles of the angles θ_i should be smooth enough, and the angles $\theta_{i,i-1}$ and $\theta_{i,i+1}$ should be sufficiently small. Then, one can assume that the distortion does not give rise to any change in the orientational order within each layer of the sample (no changes in values of the local orientational order parameters s_i), and changes in its free energy are caused by only small changes ΔV_i in one-particle pseudo-potentials (5) and (6) associated with the small rotation of the local director $\vec{n}_i$ with respect to the local directors $\vec{n}_{i-1}$ and $\vec{n}_{i+1}$ of its two neighboring layers. For the first layer, change in the one-particle pseudopotential $V_1(\vartheta_1)$ is also caused by the rotation of its local director $\vec{n}_1$ with respect to the normal $\vec{\nu}$ to the substrate surface. If it is also assumed that an axial symmetry of alignment of long molecular axes with respect to the local director $\vec{n}_i$ occurs within each ith layer, one can easily show that, in the harmonic approximation, the changes ΔV_i in the one-particle pseudopotentials $V_i(\vartheta_i)$ caused by the distortion are given by the following expressions:

$$\Delta V_1 = \tfrac{1}{2}V_0\left(\tfrac{3}{2}\cos^2\vartheta_1 - \tfrac{1}{2}\right)[s_2\theta_{1,2}^2 + 3(W_0/V_0)\theta_1^2], \tag{12}$$

$$\Delta V_{2\le i\le N-1} = \tfrac{1}{2}V_0\left(\tfrac{3}{2}\cos^2\vartheta_i - \tfrac{1}{2}\right)[s_{i-1}\theta_{i,i-1}^2 + s_{i+1}\theta_{i,i+1}^2], \tag{13}$$

$$\Delta V_N = \tfrac{1}{2}V_0\left(\tfrac{3}{2}\cos^2\vartheta_N - \tfrac{1}{2}\right)s_{N-1}\theta_{N,N-1}^2, \tag{14}$$

and corresponding changes in the free energies F_i of layers of the NLC sample are

$$\Delta F_1 = \tfrac{1}{4}N_iV_0[s_1s_2\theta_{1,2}^2 + 6(W_0/V_0)s_1\theta_1^2], \tag{15}$$

$$\Delta F_{2\le i\le N-1} = \tfrac{1}{4}N_iV_0(s_is_{i-1}\theta_{i,i-1}^2 + s_is_{i+1}\theta_{i,i+1}^2), \tag{16}$$

$$\Delta F_N = \tfrac{1}{4}N_iV_0s_Ns_{N-1}\theta_{N,N-1}^2. \tag{17}$$

Finally, assuming that the local directors of all molecular layers of the distorted sample belong to the same plane, we can rewrite Eqs. (15)–(17) in the following form:

$$\Delta F_1 = \tfrac{1}{4}N_iV_0[s_1s_2(\theta_2 - \theta_1)^2 + 6(W_0/V_0)s_1\theta_1^2], \tag{18}$$

$$\Delta F_{2\le i\le N-1} = \tfrac{1}{4}N_iV_0[s_is_{i-1}(\theta_i - \theta_{i-1})^2 + s_is_{i+1}(\theta_{i+1} - \theta_i)^2], \tag{19}$$

$$\Delta F_N = \tfrac{1}{4}N_iV_0s_Ns_{N-1}(\theta_N - \theta_{N-1})^2. \tag{20}$$

We can consider the angles θ_i $(i=1,N-1)$ as "external parameters" and, for a given value of the angle θ_N, these angles can be determined by minimizing the total change $\Delta F = \Sigma_{i=1}^{N}\Delta F_i$ in the free energy of the NLC sample with respect to each of them. This procedure leads to the following set of equations:

$$3(W_0/V_0)s_1\theta_1 - s_1s_2(\theta_2 - \theta_1) = 0,$$

$$s_is_{i-1}(\theta_i - \theta_{i-1}) - s_is_{i+1}(\theta_{i+1} - \theta_i) = 0, \quad 2 \le i \le N-1,$$

$$s_{N-2}s_{N-1}(\theta_{N-1} - \theta_{N-2}) - s_{N-1}s_N(\theta_N - \theta_{N-1}) = 0, \tag{21}$$

which has the solution

$$\theta_1 = \theta_N/(1 + K^*), \tag{22}$$

$$\theta_{2\le k\le N-1} = \theta_1\left(1 + \sum_{i=1}^{k-1} K_i^*\right), \tag{23}$$

$$K_i^* = 3(W_0/V_0)s_1/(s_is_{i+1}), \tag{24}$$

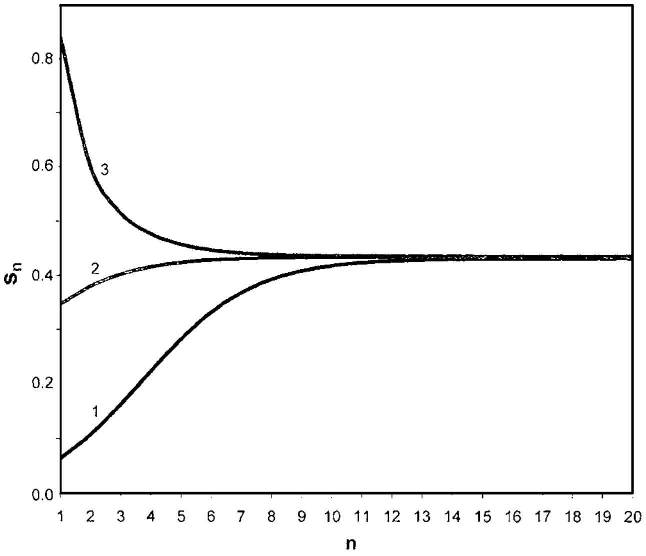

FIG. 1. Dependence of the local orientational order parameter s_n on the distance from the substrate surface (the layer number n). $T^*=0.22$. (1) $W_0/V_0=0.01$; (2) $W_0/V_0=0.1$; (3)$W_0/V_0=1$.

$$K^* = \sum_{i=1}^{N-1} K_i^*. \tag{25}$$

In this solution we can use the values of the local orientational order parameters s_i obtained from the self-consistent equations (7) for the undistorted NLC sample.

III. RESULTS OF NUMERICAL CALCULATIONS AND DISCUSSION

First of all, we have calculated the local order parameter profiles s_i for the undistorted NLC sample composed of $N = 500$ molecular layers. The results of these calculations performed at the reduced temperature $T^*=0.22$, which is very close to the first order isotropic-NLC phase transition temperature T_{IN}^* (according to the theories of McMillan and Mayer-Saupe's [41–43], $T_{IN}^*=0.2202$) for cases of strong $(W_0/V_0=1)$, weak $(W_0/V_0=0.1)$, and very weak $(W_0/V_0 = 0.01)$ anisotropic interactions between NLC molecules and the solid substrate surface, are shown in Fig. 1. It is seen that, in the case of very weak NLC-substrate anisotropic interactions, values of the local orientational order parameters near the substrate surface are significantly lower than those in the NLC bulk. In the case of a weak NLC-substrate anisotropic interactions, the orientational order at the substrate surface is only slightly lower than in the NLC bulk, and strong anisotropic interactions between NLC molecules and the solid substrate surface leads to values of the local orientational order parameters near the substrate surface almost twice as high as those in the NLC bulk.

Then, values of the local orientational order parameters s_i calculated for the undistorted NLC sample were used in the calculation of the angles θ_i which determine a deviation of the local directors $\vec{n}_i$ in the distorted sample from their initial homeotropic alignment. The profiles of these angles for strong and weak NLC-substrate anisotropic interactions, cor-

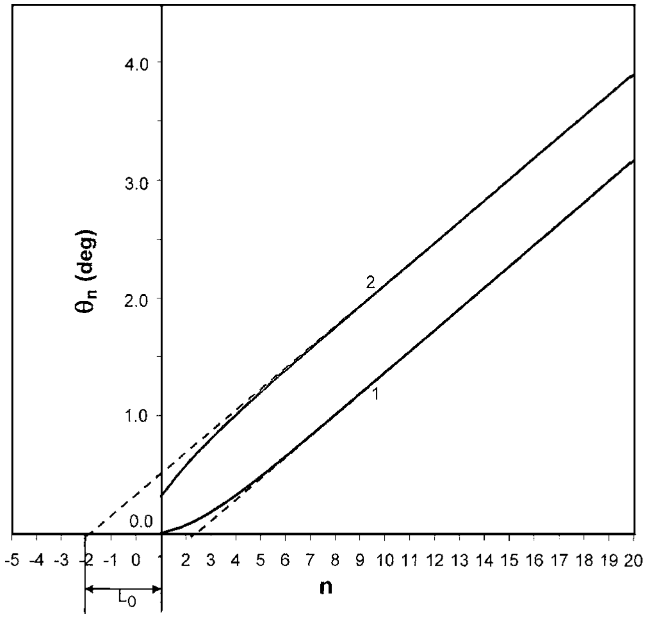

FIG. 2. The angle θ_n profiles in the NLC sample in a contact to the substrate surface. $T^*=0.22$. (1) $W_0/V_0=1$; (2) $W_0/V_0=0.1$.

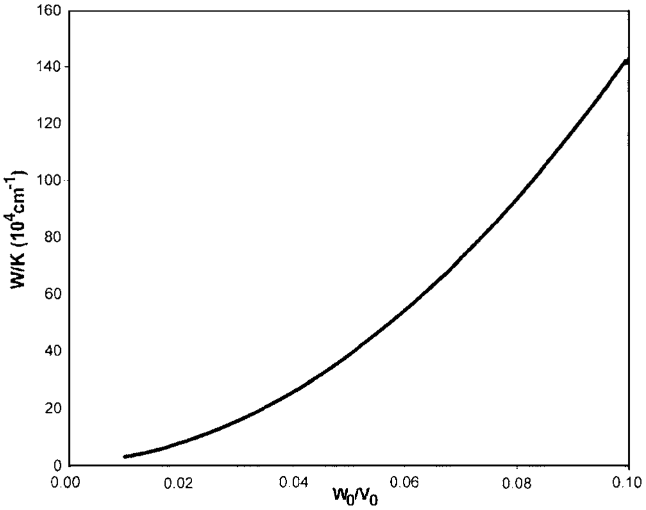

FIG. 4. Dependence of the ratio W/K on the ratio W_0/V_0. $T^*=0.22$, $l_0=2.5$ nm.

responding to curves 3 and 2, respectively, in Fig. 1, are shown in Fig. 2, whereas analogous profile for very weak NLC-substrate anisotropic interactions, corresponding to curve 1 in Fig. 1, is shown in Fig. 3. From Fig. 2 one can see that, in the case of the strong NLC-substrate anisotropic interaction (curve 1), the angle θ_1 in the first layer of the sample is equal to nearly zero, i.e., the "rigid" NLC-substrate surface anchoring occurs [1,2], and the distortion imposed on the NLC sample by a certain external action cannot penetrate into the first molecular layer of the sample. In the case of the weak NLC-substrate anisotropic interaction (Fig. 2, curve 2), though, the angle θ_1 is different from zero; it is very small ($\sim 0.5°$), and the corresponding correlation length L_0 is equal to only three molecular lengths, i.e., ~ 7 nm. If, in the relation $L_0=K/W$ (in case of the homeotropic orientation $K=K_{33}$), do we set $K\sim 10^{-6}$ dyn (10^{-11} N) (a typical value of the elastic constant K_{33} for NLCs [29,30]), then it is easily seen that this extrapolation length L_0 should correspond to $W\sim 1.4$ erg/cm^2 (1.4×10^{-3} J/m^2). So, even when the constant W_0 of the NLC-substrate surface anisotropic interaction is ten times smaller than the constant V_0 of the anisotropic intermolecular interaction in NLC, we obtain the coefficient of anchoring energy W corresponding to the case of strong anchoring. This result is in complete agreement with an assertion presented in Ref. [32] according to which the strong anchoring does not imply necessarily an existence of strong orienting action of the substrate surface on NLC on a microscopic level. Only in the case of the very weak NLC-substrate anisotropic interaction (Fig. 3), do we have a noticeable value ($\sim 14°$) of the angle θ_1, which determines the deviation of the local director $\vec{n}_1$ in the first molecular layer

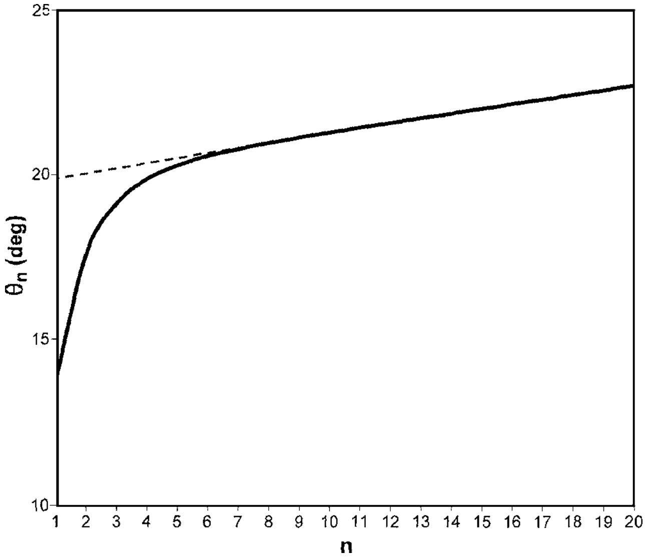

FIG. 3. The angle θ_n profile for $W_0/V_0=0.01$.

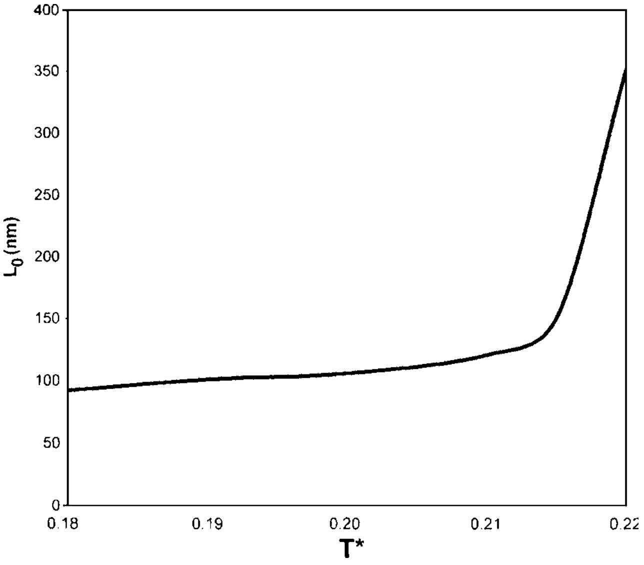

FIG. 5. Temperature dependence of the anchoring extrapolation length L_0 for $W_0/V_0=0.01$. $l_0=2.5$ nm.

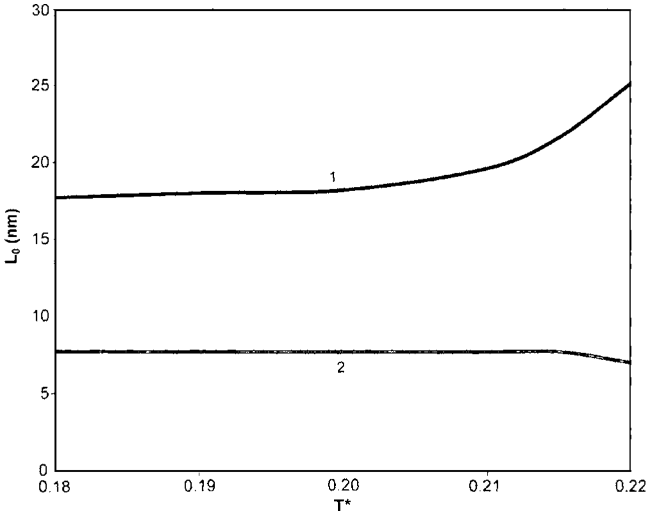

FIG. 6. Temperature dependence of the anchoring extrapolation length L_0 for W_0/V_0=0.05 (curve 1) and W_0/V_0=0.1 (curve 2). l_0 =2.5 nm.

of the NLC sample from easy axis of alignment, and the macroscopic anchoring extrapolation length $L_0 \sim 350$ nm (not shown in Fig. 3).

In order to investigate a relation between the ratio W_0/V_0, which in the framework of the model offered here, characterizes the NLC-substrate surface anisotropic interaction on a microscopic level, and the coefficient W, which characterizes the orienting action of the substrate surface on the NLC on a macroscopic level, we calculated the angles θ_i for different values of the ratio W_0/V_0 at the constant reduced temperature T^*=0.22 of the NLC sample. For each profile of these angles, we determined the extrapolation length L_0 (in all calculations the molecular length l_0 was assumed to be 2.5 nm that is a typical value for LCs [29,30]), and, hence, the ratio W/K. The results of these calculations for W_0/V_0 ranging from 0.01 to 0.1 are presented in Fig. 4. Then, if we know the value of the elastic constant K ($\sim 10^{-6}$ dyn, the curve depicted in this figure allows us to find the relation between the ratioW_0/V_0 and the coefficient W. So, one can find, for example, that the anchoring energy coefficient $W \sim 10^{-2}$ erg/cm^2 ($\sim 10^{-5}$ J/m^2) corresponds to $W_0/V_0 \sim 0.01$, $W \sim 10^{-1}$ erg/cm^2 ($\sim 10^{-4}$ J/m^2) corresponds to $W_0/V_0 \sim 0.03$, and $W \sim$ erg/cm^2 ($\sim 10^{-3}$ J/m^2) corresponds to $W_0/V_0 \sim 0.08$.

The results obtained also enable us to establish a relation between the local orientational order parameter profiles in the interfacial NLC region and the anchoring energy coefficient W. Comparing the results of the calculations presented in Figs. 1–4, one can find that, in the case of the weak anchoring ($W \sim 10^{-2}$ erg/cm^2), the local orientational order parameters near the substrate surface are significantly smaller than those in the NLC bulk, the strong anchoring ($W \sim$ erg/cm^2) corresponds to such local orientational order parameter profiles when the orientational order in the interfacial region is comparable with that in the bulk nematic phase, and, finally, when the orientational order near the substrate surface is much higher than that in the NLC bulk, the rigid NLC-substrate surface anchoring occurs.

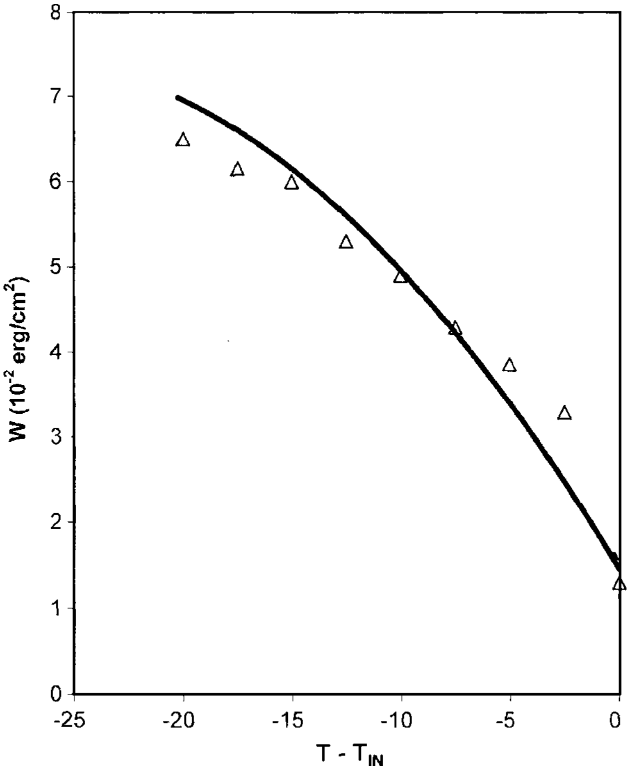

FIG. 7. Temperature dependence of the anchoring energy coefficient W for NLC MBBA. Δ, experimental points from Ref. [45].

We have also calculated the temperature dependence of the anchoring extrapolation length L_0 at different values of the ratio W_0/V_0. The results of these calculations, for W_0/V_0=0.01, 0.05, and 0.1, are shown in Figs. 5 and 6. From Figure 5 it follows that, in the case of weak anchoring (W_0/V_0=0.01, $W \sim 10^{-2}$ erg/cm^2), lowering the temperature of the NLC sample leads to a significant (more than three times) decay of the anchoring extrapolation length L_0 as compared to its value close to the isotropic-nematic phase transition temperature T^*_{IN}, and this decay is very fast in a vicinity of the transition temperature, and the extrapolation length L_0 lowers insignificantly enough with further decreasing temperature. According to Fig. 6 (curve 1), for W_0/V_0 =0.05 ($W \sim 3 \times 10^{-1}$ erg/cm^2), the lowering temperature of the NLC sample results in a much less significant decrease in the anchoring extrapolation length L_0 (from $L_0 \sim 25$ nm near T^*_{IN} to $L_0 \sim 18$ nm at T^*=0.18). An essential part of this decay occurs also in the range close to the isotropic-nematic phase transition temperature, and further lowering the temperature does not lead to any noticeable decrease in L_0. This result is in good agreement with experimental data [44] on both magnitude and behavior of the anchoring extrapolation length L_0. Finally, for W_0/V_0=0.1 ($W \sim$ erg/cm^2), the magnitude of the extrapolation length L_0 is equal to about 7 nm, and this value is nearly temperature independent.

In conclusion, we calculated the temperature dependence of the anchoring energy coefficient W for the concrete NLC material MBBA in a contact to the substrate surface covered by a surfactant inducing the homeotropic alignment in the NLC sample, and the results obtained were compared with experimental data [45]. First of all, we used the experimental value $W=1.3\times10^{-2}$ erg/cm^2, which was measured near the isotropic-nematic phase transition temperature T_{IN} [for MBBA $T_{IN}=318$ K (45 °C)], as well as value of the elastic constant $K=K_{33}\approx4.5\times10^{-7}$ dyn [29] typical for NLC MBBA at the same temperature. It appeared that the corresponding value of the anchoring extrapolation length $L_0=K/W$ can be obtained from our microscopic model at $W_0/V_0\approx0.01$. Using this value of the ratio W_0/V_0, we have calculated the temperature dependence of the anchoring extrapolation length $L_0=K/W$, and then, taking into account that the elastic constant K should be proportional to s_b^2, where s_b is the orientational order parameter in the NLC bulk, we have obtained the temperature dependence of the coefficient W shown in Fig. 7. The experimental points from Ref. [45] are also presented in this figure. It is easily seen that an agreement between our theoretical results and the experimental data is well enough.

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