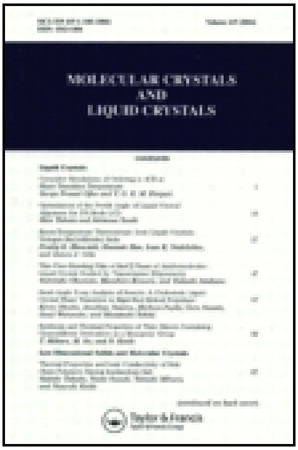

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Influence of Surface Elasticity on Periodic Splay-Twist Freedericksz Transition in a Nematic Cell

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On the basis of local stability analysis we have studied how the surface-like elastic terms influence periodic splay-twist Freedericksz transition in a nematic liquid crystal (NLC) sandwiched between two parallel plates. It is assumed that the planar anchoring favored at both walls and magnetic field is normal to the confining surfaces. Assuming stability of the director ground state in the zero field limit, restrictions on elastic constants are obtained. The critical ratio of the twist and splay elastic constants is calculated as a function of K_{24}. It is found that there is a critical value of K_{24}, such that the transition is suppressed under K_{24} exceeds this value. Effects of anchoring energy and the K_{13} - term are discussed.

Keywords: surface elasticity; periodic splay-twist Freedericksz transition

INTRODUCTION

It is known[1] that for nematic with a ratio of the twist and splay Frank elastic constants, $r = \frac{K_{22}}{K_{11}}$, smaller than a critical value, the usual homogenous splay Freedericksz transition is replaced by a spatial periodic splay-twist distortion. If such a NLC is arranged in a cell with planar anchoring favored at both walls is subjected to a magnetic field, then above a certain threshold the invariance of the transition is broken along the axis normal to the undistorted director in the boundary plane: the equilibrium configuration of the director in the sample assumes now a static spatial periodicity characterized by a wave number, $k = \frac{2\pi}{L}$, where L is the spatial period of the structure. The basic reason for the occurence of the periodic distortion is that a mixed distortion, consisting of a twist superimposed to a small splay, is favored in energy over a simple but pronounced splay under the elastic contant associated with splay is much larger than the one associated with twist (a NLC composed by very long molecules).

In subsequent papers[2–6] the effect of weak anchoring and or of different external fields on the transition to the splay-stripes is described. Next step in trying to address the problem in the case of finite anchoring is to consider the role of surface elasticity. In other words, this raises the question as to influence of two gradient terms in the surface free energy expansion, known als the K_{24}-term and the K_{13}-term, on the transition.

The K_{13}-term is known to cause fundamental difficulties in the theory[7]. There are two competing theories that offer the solution to the K_{13}-problem. The first was put forward by Pergamenshchik[8], the other one by Faetti[9]. The procedure we adopt is to take the term into account by making use the theory of Ref.[8], so that the case with $K_{13} = 0$ correspond to the approach by Faetti. (It can be shown that within the latter approach we just need to renormalize K_{24}.) Estimates reported in Ref.[10] will be used to discuss effects due to K_{13}.

The organization of the paper is as follows. In Sec. 2, by making use of the symmetry of the problem, we derive a set of key equations. In Sec. 3, starting from the assumption that the ground director state of NLC not subjected to an external fiel is stable, we obtain the restriction on K_{24}. Sec.4 starts with the case of strong anchoring boundary conditions. It is found that the K_{24} plays the dual role in the problem: the critical value of r is an increasing function of K_{24}, but, due to the restriction imposed on K_{24}, there is a critical calue of K_{24} above which the transition is inhibited. The dependence of the critical value of K_{24} on the anchoring energy is calculated for various valued of K_{13}. Concluding remarks are given in Sec. 5.

STABILITY ANALYSIS

Let us onsider NLC sandwiched between two identical parallel plates, $z = \frac{d}{2}$, and $z = -\frac{d}{2}$, assuming the vector of easy orientation is directed along the x-axis at both substrates and the magnetic field is applied along the z-axis. The NLC director field can be expressed in terms of two angles, Θ and Φ:

$$\vec{n} = \sin\Theta\cos\Phi \cdot \vec{e}_x + \sin\Theta\sin\Phi \cdot \vec{e}_y + \cos\Theta \cdot \vec{e}_z \tag{1}$$

where both of the angles are functions of y and z.

The planar director configuration can be obtained form Eq. 1 by setting $\Phi = 0$ and $\Theta = \frac{\pi}{2}$. In what follows θ and ϕ stand for small deviations of the angles from their above values.

The K_{24}-term and the K_{13}-term can be taken in the form:

$$F_{24} = -\frac{K_{24}}{2}\int_{\nu} \mathrm{d}\nu \, \mathrm{div}\,(\vec{n}\,\mathrm{div}\,\vec{n} + \vec{n} \times \,\mathrm{curl}\,\vec{n}) \tag{2}$$

$$F_{13} = \frac{K_{13}}{2}\int_{\nu} \mathrm{d}\nu \, \mathrm{div}\,(\vec{n}\,\mathrm{div}\,\vec{n}) \tag{3}$$

Then, by making use of the standard Oseen-Frank free energy expression and Eqs. 1-3, the second-order variation of the free energy functional can be derived as a bilinear part of the free energy per unit length in θ and ϕ. The result reads

$$\begin{aligned}\delta^2 F = \frac{K_{11}}{2} &\int \mathrm{d}z\mathrm{d}y \left(\left(\phi'_y - \theta'_z\right)^2 + r\left(\phi'_z + \theta'_y\right)^2 - \left(q_1\theta\right)^2\right) + \\ &+ \int \mathrm{d}y \left\{ \left(\frac{W_\theta}{2}\theta^2 + \frac{W_\phi}{2}\phi^2\right)\Big|_{z=\pm d/2} - K_{24}\phi\,\theta'_y\Big|_{-d/2}^{d/2} \right\} + \\ &+ \frac{K_{13}}{2}\int \mathrm{d}y \left\{ \phi\theta'_y + \theta\theta'_z\Big|_{-d/2}^{d/2} \right\}\end{aligned} \tag{4}$$

where $q_i^2 = \frac{\chi_a H^2}{K_{ii}}$ and W_θ (W_ϕ) is the tilt (twist) anchoring strength.

Since we are looking for transverse periodicity along the y-axis, the angle fluctuations are periodic funcions of y and can be expanded into Fourier series:

$$\theta(z,y) = L^{-1/2}\sum_{n=-\infty}^{\infty} \theta_n(z)\exp(ik_n y) \tag{5}$$

$$\phi(z,y) = L^{-1/2} \sum_{n=-\infty}^{\infty} \phi_n(z) \exp(ik_n y), \quad k_n = \frac{2\pi n}{L} \tag{6}$$

so that each fluctuation harmonics contribute independently to the second-order variation of the free energy per stripe of width L. Introducing new Fourier amplitudes $\phi_n = A_n - i\tilde{A}_n$ and $\theta_n = \tilde{B}_n - iB_n$, the latter can be written as a sum of the contributaions $\delta^2 F_n$ that depend on A_n and B_n. (The contributions depending on $\tilde{A}_n$ and $\tilde{B}_n$ are of the same form and can be eliminated from the consideration.)

Eqs. 4-6 provide the following Euler-Lagrange equations:

$$\begin{cases} B_n'' + (q_1^2 - rk_n^2)B_n + k_n(r-1)A_n' &= 0 \\ rA_n'' - k_n^2 A_n - k_n(r-1)B_n' &= 0 \end{cases} \tag{7}$$

with linearized boundary conditions:

$$\begin{cases} \pm\left(K_{22}A_n' + k_n(K_{24} - K_{22} - K_{13}/2)B_n\right) + W_\phi A_n\big|_{z=\pm\frac{d}{2}} &= 0 \\ \pm\left((K_{11}+K_{13})B_n' + k_n(K_{24} - K_{11} - \frac{K_{13}}{2})A_n\right) + W_\theta B_n\big|_{z=\pm\frac{d}{2}} &= 0 \end{cases} \tag{8}$$

where the prime stands for the derivative with respect to z.

Note that Eqs. 7,8 indicate the appearance of null eigenvalue of the Sturm-Liouville problem associated with the linearized Euler-Lagrange equations for the director field, so that the condition for the boundary-value problem (7),(8) to have a nontrivial solution provides the dependence of the critical field, or q_1, on wave number, k_n.

There are four integration constants which enter the general solution of Eq. 7, so that Eq. 8 implies a 4x4-determinant is equal to zero. But the problem has the following mirror symmetry: if a pair of functions forms a solution of Eq. 7 and on of them is an odd (even) function, then another one is an even (odd) function. To take advantage of the above symmetry let us rewrite the boundary conditions in terms of new amplitudes:

$$a_\pm = \frac{1}{2}\left[A_n\left(\frac{d}{2}\right) \pm A_n\left(-\frac{d}{2}\right)\right], \quad b_\pm = \frac{1}{2}\left[B_n\left(\frac{d}{2}\right) \pm B_n\left(-\frac{d}{2}\right)\right]$$

$$a_\pm' = \frac{d}{4}\left[A_n'\left(\frac{d}{2}\right) \pm A_n'\left(-\frac{d}{2}\right)\right], \quad b_\pm' = \frac{d}{4}\left[B_n'\left(\frac{d}{2}\right) \pm B_n'\left(-\frac{d}{2}\right)\right]$$

Due to the symmetry, the fundamental system of solutions to Eq. 7 can be chosen in such a way that

$$\begin{pmatrix} a_+ \\ b_- \end{pmatrix} = P_1 \begin{pmatrix} C_1 \\ D_1 \end{pmatrix}, \quad \begin{pmatrix} a'_- \\ b'_+ \end{pmatrix} = Q_1 \begin{pmatrix} C_1 \\ D_1 \end{pmatrix} \tag{9}$$

$$\begin{pmatrix} a_- \\ b_+ \end{pmatrix} = P_2 \begin{pmatrix} C_2 \\ D_2 \end{pmatrix}, \quad \begin{pmatrix} a'_+ \\ b'_- \end{pmatrix} = Q_2 \begin{pmatrix} C_2 \\ D_2 \end{pmatrix} \tag{10}$$

where P_i and Q_i are matrixes defined by the fundamental system of solutions; C_i and D_i are the integration constants. Eqs. 9-10 give the boundary conditions in the form

$$\det \left| \begin{pmatrix} r & 0 \\ 0 & 1+q_{13} \end{pmatrix} Q_i + \begin{pmatrix} w_\phi & x(q_{24}-\frac{q_{13}}{2}-r) \\ x(q_{24}-\frac{q_{13}}{2}-1) & w_\theta \end{pmatrix} P_i \right| = 0 \tag{11}$$

where $x = \frac{k_n d}{2}$, $w_{\phi,\theta} = \frac{W_{\phi,\theta} d}{2K_{11}}$, $q_{ij} = \frac{K_{ij}}{K_{11}}$.

Eq. 11 with $i = 1$ gives an equation to find the x-dependence of the critical field under instability governed by even fluctuations of the azimuth angle and odd fluctuations of the tilt angle. In the case of $i = 2$ we have the equation for the instability threshold determined by odd fluctuations in the azimuth angle and even fluctuations in the tilt angle.

STABILITY OF THE GROUND STATE

In the previous section we have tacitly assumed stability of the director ground state, $\vec{n}_0 = \vec{e}_x$, in the absence of the destabilizing magnetic field. It implies no so-called anomalously deformed director states. As a consequence, elastic constants cannot take arbitrary values and stability of the ground state can be used to get restrictions on them.

To this end one has to find general solution of Eq. 7 with $q_1 = 0$ (H=0) and obtain the expressions for P_i and Q_i from Eqs. 9-10. The result reads

$$P_2 = \begin{pmatrix} \sinh x + x\rho\cosh x & -x\rho\cosh x \\ x\rho\sinh x & \cosh x - x\rho\sinh x \end{pmatrix} \tag{12}$$

$$Q_2 = x \begin{pmatrix} (1+\rho)\cosh x + x\rho\sinh x & -\rho\cosh x - x\rho\sinh x \\ \rho\sinh x + x\rho\cosh x & (1-\rho)\sinh x - x\rho\cosh x \end{pmatrix} \tag{13}$$

where $\rho = \frac{1-r}{1+r}$ and $P_1(Q_1)$ can be derived from Eq. 12 (Eq. 13) by making substitution: $\sinh x \leftrightarrow \cosh x$.

From Eq. 11 with $i = 2$ (the case of $i = 1$ leads to the same restriction) the condition for the ground state configuration to be unstable can be obtained in the form:

$$a_3 x^3 + a_2 x^2 + a_1 x + a_0 = 0 \tag{14}$$

where

$$\begin{aligned} a_3 &= (q_{24}^2 - q_{13}^2/4)\rho\left(\tanh^2 x - 1\right) ; \\ a_2 &= \left(-q_{24}^2 + \frac{2r}{(r+1)} q_{24}(q_{13}+2) + q_{13}^2 \frac{(1-3r)}{(4+4r)}\right) \tanh x ; \\ a_1 &= w_\phi w_\theta \rho \left(1 - \tanh^2 x\right) + w_\phi \tanh^2 x (1-\rho) + r w_\theta (1+\rho) ; \\ a_0 &= w_\phi w_\theta \tanh x . \end{aligned}$$

Eq. 14 yields the stability condition: $a_2 > 0$ and the restriction on K_{24}:

$$\frac{r(2+q_{13}) - D^{1/2}}{1+r} < q_{24} < \frac{r(2+q_{13}) + D^{1/2}}{1+r} \tag{15}$$

$$D = 4r^2(1+q_{13}) + q_{13}^2(1-r)^2/4$$

In the case of $K_{13} = 0$ we have

$$0 < q_{24} < \frac{4r}{r+1} \qquad \text{or} \qquad 0 < K_{24} < \frac{4K_{22}}{K_{22}+K_{11}} \tag{16}$$

Another form of Eq. 16 is

$$r > \frac{q_{24}}{4 - q_{24}}, \quad q_{24} \in (0,4) \tag{17}$$

Since the right hand side of Eq. 17 is an increasing function of q_{24}, we readily arrive at the conclusion that if the right hand side is greater than the critical value of r, then no periodic director deformation can occur. In other words, the K_{24}-term suppresses the periodic splay-twist Freedericksz transition provided that K_{24} is sufficiently large. But is should be emphasized that the issue is virtually more complicated, since the critical calue of r, in its turn, depends on K_{24}. We shall extend on this subject in

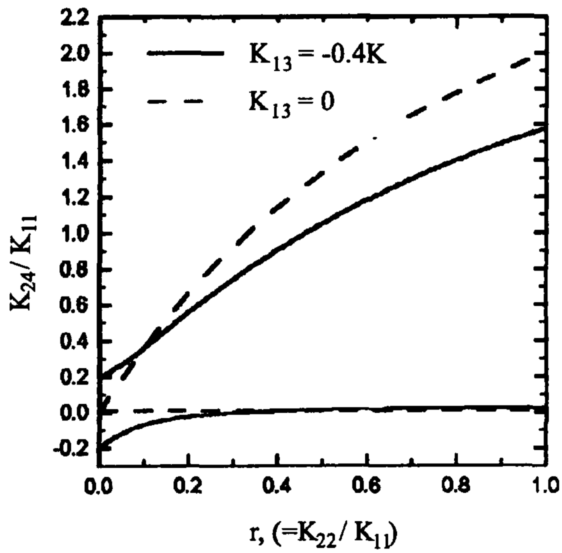

FIGURE 1 Stability region of the NLC director ground state in the $r - q_{24}$ plane. The region is enclosed by solid (dashed) lines for $K_{13} = -0.4K_{11}$ ($K_{13} = 0$)

Sec.4. Note that, in the one-constant approximation, Eq. 16 was obtained in Ref.[11] for NLC confined in cylindrical geometry.

According to Ref.[10], where 5CB submicron films were studied to verify the status of the K_{13}-term, the relevant constants can be estimated as: $K_{13} \approx -0.4K_{11}$, $r \approx 0.623$ and $K_{24} \approx -0.2K_{11}$ (or $K_{24} \approx 1.8K_{11}$). Referring to Fig. 1, it is clearly seen that the reported values are outside the region where the NLC director ground state is stable.

PERIODIC PATTERN FORMATION AND SURFACE ELASTICITY

In this section we consider conditions for the periodic stripes to appear, so that or prime interest is in the critical values of r and q_{24}.

In order to facilitate subsequent discussion we start from the case when the strong anchoring is applied to both substrates, $W_{\theta,\phi} \to \infty$. Then, instead of Eq. 11, we have

$$\det P_1 = 0, \quad \text{or} \quad \det P_2 = 0 \ . \tag{18}$$

Let us consider Eq. 18 at smaller wave numbers: $k_n < q_2$. After solving of Eq. 7 it is straightforward to derive the needed matrixes in the form:

$$P_2 = \begin{pmatrix} -l_1 \sin(au_2) & \sinh(bu_2) \\ \cos(au_2) & l_2 \cosh(bu_2) \end{pmatrix} ; \tag{19}$$

$$Q_2 = u_2 \begin{pmatrix} -al_1 \cos(au_2) & b \cosh(bu_2) \\ -a \sin(au_2) & bl_2 \sinh(bu_2) \end{pmatrix} ; \tag{20}$$

where

$$l_1 = \frac{a\chi(1-r)}{ra^2+\chi^2}, \quad l_2 = \frac{b\chi(1-r)}{b^2+r(1-\chi^2)}; \quad \chi = \frac{k_n}{q_2}; \quad u_i = \frac{q_i d}{2}; \tag{21}$$

$$a^2 = \frac{1}{2}\left[\left(r^2+4\chi^2(1-r)\right)^{1/2} + r - 2\chi^2\right] ; \tag{22}$$

$$b^2 = \frac{1}{2}\left[\left(r^2+4\chi^2(1-r)\right)^{1/2} - r + 2\chi^2\right] ; \tag{23}$$

and substituting: $\sin(au_2) \to -\cos(au_2)$, $\cos(au_2) \to \sin(au_2)$, $\sinh(bu_2) \leftrightarrow \cosh(bu_2)$ into Eq. 19 (Eq. 20) gives $P_1(Q_1)$.

In what follows it is convenient to take χ, which is the product of the wave number and the magnetic coherence length, as an independent dimensionless parameter, assuming that the magnetic fiel is controlled by the dimensionless parameter u_2. So, we need to calculate the dependence of the critical value of u_2, u_c, on χ.

To do this let us consider Eq. 20 with $i = 2$ that gives the following equation for u_c:

$$\cot(au_2) = -\chi^2 \gamma\, a\, b \coth(b\, u_c) \tag{24}$$

where

$$\gamma = \frac{(1-r)^2}{(ra^2+\chi^2)(b^2+r(1-\chi^2))} \ .$$

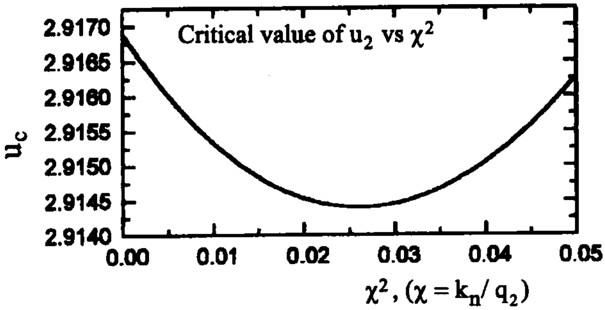

FIGURE 2 The χ-dependence of the treshold u_c, in the strong anchoring limit at $r = 0.29$.

An immediate consequence of Eq. 24 is: $\sqrt{r}u_c(0) = \pi/2$, that is to say Eq. 24 gives the treshold of the usual homogeneous Freedericksz transition at $\chi = 0$. Note that u_c virtually depends on χ^2 and we can take the condition:

$$\left.\frac{du_c}{d(\chi^2)}\right|_{\chi=0} < 0$$

as a condition for the periodic transition to occur. After differentiating of Eq. 24 and making some algebraic manipulations, we get the condition for the appearance of the periodic director distortions:

$$(r-1)^2 - \frac{\pi^2}{8}(1-2r) < 0 \tag{25}$$

Eq. 25 provides the well-known result[2,3]:

$$r < r_c = 1 - \frac{\pi^2}{8} + \sqrt{\frac{\pi^2}{8}\left(\frac{\pi^2}{8} - 1\right)} \approx 0.30325\ . \tag{26}$$

Referring to Fig. 2, the treshold u_c reaches its least value at the nonzero wave number, $k \approx 0.93d^{-1}$ for $r_c > r = 0.29$.

Now we proceed with study of how the K_{24}-term affects the above result. The starting point of our analysis is Eq. 11 with $i = 2$ and the matrixes defined in Eqs. 19,20, so that the equation for the threshold reads

$$\cot(au_2) = \frac{A}{B} \tag{27}$$

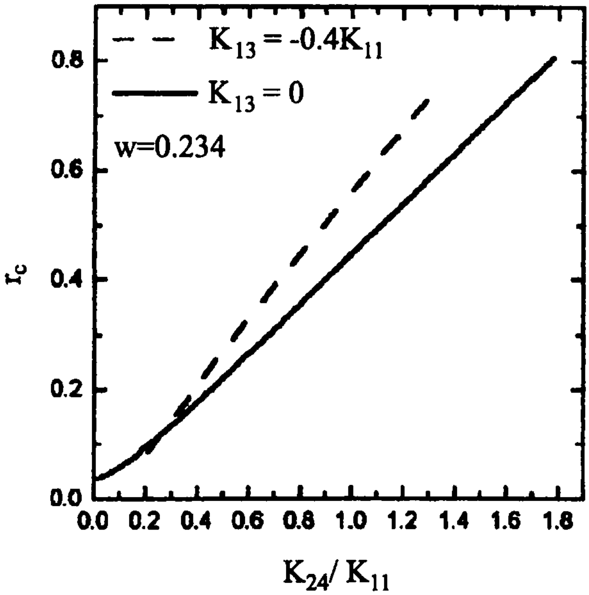

FIGURE 3 Dependence of the critical ratio r_c on K_{24} at $w = 0.234$ for $K_{13} = 0$ (solid line) and $K_{13} = -0.4K_{11}$ (dashed line).

where

$$
\begin{aligned}
A &= u_2^2 \coth(bu_2) \left[a(1+q_{13}) + \chi^2 l_1 (q_{24} - q_{13}/2 - 1)\right] \cdot \\
&\quad \cdot \left[rb + \chi^2 l_2 (q_{24} - q_{13}/2 - r)\right] + \\
&\quad + w_\phi \left[a(1+q_{13})u_2 - \chi^2 l_1 l_2 (w_\theta \coth(bu_2) + bu_2(1+q_{13}))\right] , \\
B &= w_\theta \left[w_\phi + ru_2 \coth(bu_2)(b + \chi^2 a l_1 l_2)\right] - \\
&\quad - (\chi u_2)^2 \left[q_{24} - r(1+al_1) - q_{13}/2\right] \cdot \\
&\quad \cdot \left[b(1+q_{13})l_2 + q_{24} - q_{13}/2 - 1\right]
\end{aligned}
\tag{28}
$$

Fig. 3 shows the dependence of the critical value of r_c on q_{24}. It is seen that r_c is an increasing function of K_{24}. On the other hand, Eqs. 16,17 imply that there is a critical value of q_{24}, q_c, such that the periodic transition cannot occur provided that $q_{24} \geq q_c$. From Eq. 17 it is clear that

$$q_c = \frac{4r_c}{r_c + 1} \; . \tag{29}$$

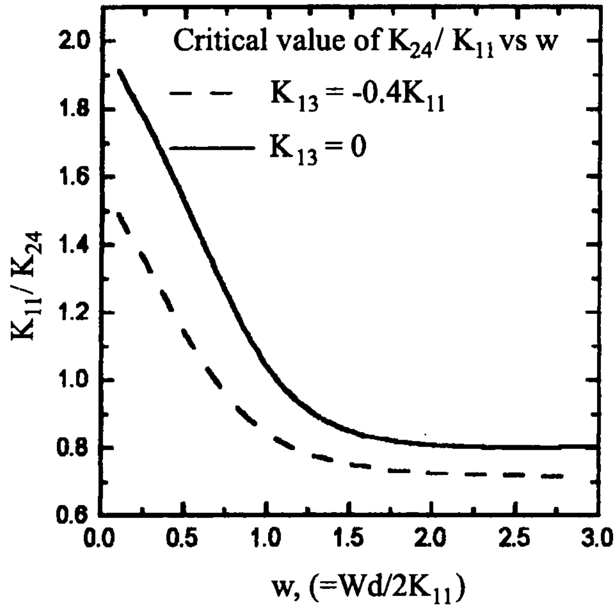

FIGURE 4 The w-dependence of the critical value of K_{24} at $K_{13} = 0$ (solid line) and $K_{13} = -0.4K_{11}$ (dashed line).

Since r_c, in its turn, depends on q_c, the latter is the equation to find the critical value of q_{24}. It is of interest to see how the anchoring energy strength influences q_c. The dependence of q_c on the anchoring energy in the symmetric case, where $w_\theta = w_\phi = w$, is shown in Fig. 4. In particular, the plot indicates that r_c can be greater than 0.5 at small values of w, $w \leq 0.7$. It follows that, in the presence of the K_{24}-term, 0.5 is no longer a limit value for r_c. (The existence of the above limit value was reported in Ref.[2,3]).

CONCLUSION

In this paper we have studied the effect of surface elasicity on conditions for the occurence of the periodic splay-twist Freedericksz transition. Since the critical value of r is found to be an increasing function of K_{24}, the term somehow eases the formation of the splay-stripes. But, from the other hand, the restriction imposed on K_{24} leads to the existence of its critical value above which the periodic director distortions are suppressed.

The plots presented in Figs. 3-4 show that the negative K_{13} hampers the formation of the periodic structure and the stability diagram in Fig. 1 reveals the data reported in Ref.[10] correspond to the region where the director ground state is unstable. An extended discussion of the K_{13}-problem is beyond the scope of this paper, so we just point out that the recent theoretical[12,13] and experimental[14] studies have shown the problem far from being clarified.

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