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Out of shear plane deformations in nematic liquid crystals

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The stability of the director field to deformations out of the plane of shear is examined by use of the Taylor expansion method based on catastrophe theory. For simple shear flow of nematics, the coming out of the shear plane is found for suitable surface alignment and not too high twist elastic constant. The role of these parameters is pointed out. Non-flow-aligning nematics are also considered, and results consistent with earlier reports are obtained.

1. Introduction

In recent papers [1, 2], the problem of the stability of the states induced by simple shear flow was considered. Non-flow-aligning nematics, with a negative α_3/α_2 ratio, were taken into account. In the present paper, the same problem is examined by means of the Taylor expansion method based on catastrophe theory. Attention is focused on the case of materials characterized by $\alpha_3/\alpha_2>0$, nevertheless the results for the opposite case are mentioned. In the previous paper [3], the same approach was applied to an analysis of the development of shear flow alignment, but director deformations were limited to the plane of shear. Numerical calculations [4] have been based on the same assumption. Here the director deviation from this plane is allowed and as a result the occurrence of coming out of the shear plane is found; the conditions for it are determined.

The method applied here is presented in § 2. In § 3, the particular case is considered, in which the surface alignment angle θ_1 is $-\arctan\sqrt{\alpha_3/\alpha_2}$. In § 4, the behaviour of the layer for arbitrary θ_1 and α_3/α_2 is described. Section 5 contains a short discussion of the results.

2. Method

The geometry of the system is shown in figure 1. For simple shear flow, a thin layer of nematic, characterized by Leslie coefficients α_i and elastic constants k_{ii}, is confined between two parallel plates at a distance d apart, one at rest and the other moving under the influence of constant shear stress τ. The stationary director distribution can be described by two angles, $\theta(z)$ and $\phi(z)$. The director components are:

$$n_x=\sin\phi,\quad n_y=\cos\phi\cos\theta,\quad n_z=\cos\phi\sin\theta.$$

Identical strong anchoring is assumed on both boundary surfaces: $\theta(-d/2)=\theta(d/2)=\theta_1$, $\phi(-d/2)=\phi(d/2)=0$. The simplifying assumption $\alpha_1=0$ is used.

In brief, the idea of the method adopted is as follows. The total free energy per unit area of the layer, G, is calculated. It is expressed as a function of the variables which measure the small director deviations from the initial state. This function is then expanded in a Taylor series and truncated according to rules given by catastrophe

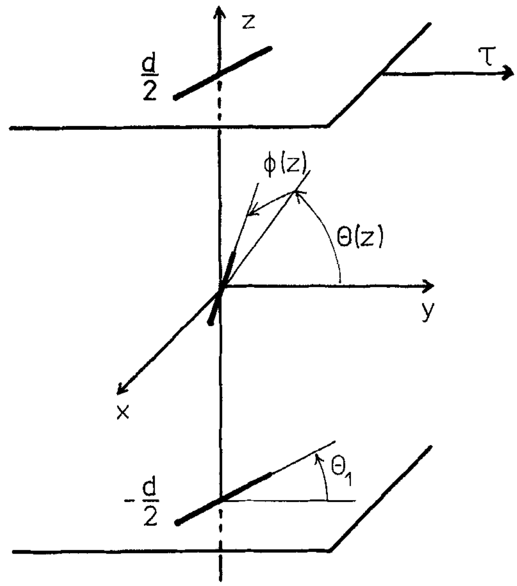

Figure 1. The geometry of the nematic layer in the simple shear flow.

theory. By minimizing this reduced form, we obtain information on the equilibrium states of the system. For application in a dissipative system this procedure should be modified. Another function, which could play the role of the energy G, should be constructed.

In the nematic layer under steady shear flow, the equilibrium director distribution results from the competition between the elastic and viscous torques, giving the resultant torque of zero. Any perturbation of this distribution requires some work to overcome the resulting torque, which tends to restore the previous equilibrium. As a result of this torque the system has the ability to do work at any perturbed state. Provided that both perturbation and relaxation are performed very slowly and along an identical path, they are related to the same (positive) value of the work (taken per unit volume):

$$g = \int \mathbf{\Gamma} \cdot d\mathbf{\Omega}, \tag{1}$$

where $d\mathbf{\Omega}$ is the elementary angular displacement vector, directed normal to the instantaneous plane of director rotation. Its minimum value, of zero, is due to the unperturbed state. Therefore it can be used to determine the equilibrium state of the system.

The purpose of this paper is to investigate the stability of the system against a small departure of the director from the shear plane. The equilibrium orientation within the shear plane can be found by taking into account the work done during the change of the angle θ, when ϕ is zero

$$g_\theta = \int_0^\theta \Gamma_\theta d\theta \bigg|_{\phi=0}, \tag{2}$$

where Γ_θ denotes the resulting torque if θ has a non-equilibrium value. Since any constant added to g is not important in further considerations of the Taylor series, we can choose a convenient range of integration, namely: from 0 to θ. If the considered deviations from the shear plane are small, then they can be described by the variable ϕ and constant θ:

$$g_\phi = \int_0^\phi \Gamma_\phi d\phi \bigg|_{\theta=\text{constant}}, \tag{3}$$

where Γ_ϕ denotes the torque tending to turn the director back to the shear plane. The work due to this departure has a minimum at $\phi=0$ if the in-plane-of-shear state is stable. The sum of both work terms

$$g = g_\theta + g_\phi, \tag{4}$$

also has therefore a minimum. If the in-plane state is unstable, then the work g_ϕ is negative and the sum does not have a minimum at $\phi=0$. The total work can be divided into two parts: the elastic part can be expressed by the Frank free energy density

$$\begin{aligned} g_{\text{elastic}} = \frac{k_{11}}{2}\bigg[& \sin^2\phi \sin^2\theta \left(\frac{\partial \phi}{\partial z}\right)^2 + \cos^2\phi\cos^2\theta\left(\frac{\partial\theta}{\partial z}\right)^2 \\ & -2\sin\phi\cos\phi\sin\theta\cos\theta\frac{\partial\phi}{\partial z}\frac{\partial\theta}{\partial z}\bigg] \\ & +\frac{k_{22}}{2}\bigg[\cos^2\theta\left(\frac{\partial\phi}{\partial z}\right)^2 + \sin^2\phi\cos^2\phi\sin^2\theta\left(\frac{\partial\theta}{\partial z}\right)^2 \\ & +2\sin\phi\cos\phi\sin\theta\cos\theta\frac{\partial\phi}{\partial z}\frac{\partial\theta}{\partial z}\bigg] \\ & +\frac{k_{33}}{2}\bigg[\cos^2\phi\sin^2\theta\left(\frac{\partial\phi}{\partial z}\right)^2 + \cos^4\phi\sin^2\theta\left(\frac{\partial\theta}{\partial z}\right)^2\bigg]. \end{aligned} \tag{5}$$

The viscous part is given by the integrals

$$g_{\text{viscous}} = -\int_0^\theta \Gamma_x\bigg|_{\phi=0} d\theta - \int_0^\phi \Gamma_{yz}\bigg|_{\theta=\text{const}} d\phi, \tag{6}$$

where

$$\Gamma_{yz} = \Gamma_y \sin\theta - \Gamma_z\cos\theta, \tag{7}$$

and Γ_x, Γ_y and Γ_z denote the components of the viscous torque vector. In the following, the angles θ and ϕ are expressed by means of two variables ξ and χ. The function

$$g = g_{\text{elastic}} + g_{\text{viscous}}, \tag{8}$$

is expanded in a Taylor series and then integrated over z. In this way the total function G per unit area of the layer is obtained, it can then be used for further analysis. Some details of the calculations of g are given in the Appendix.

3. Critical surface orientation of flow-aligning nematics

In this particular case, the flow alignment value is imposed on the surface orientation angle

$$\theta_1 = -\arctan\sqrt{(\alpha_3/\alpha_2)}. \tag{9}$$

With no shear, the director is uniform across the gap: $\theta(z)=\theta_1$. Small deformations of its distribution are assumed and they can be approximated by their first Fourier components:

$$\theta(z)=\theta_1+\xi\cos(\pi z/d), \tag{10}$$

$$\phi(z)=\chi\cos(\pi z/d). \tag{11}$$

These formulae can be used to express the approximate form of the total work per unit area of the layer, G. It represents the family of functions of two variables, ξ and χ, which is dependent on the geometrical and material constants and the shear stress. It can be expanded in a Taylor series in powers of ξ and χ in the vicinity of $\xi=0$ and $\chi=0$:

$$G=\sum_i\sum_j a_{ij}\xi^i\chi^j. \tag{12}$$

The coefficients a_{ij}, essential in further calculations, are given by:

$$a_{10}=(2\pi k_{33}/d)t(s\cos^2\theta_1-\sin^2\theta_1)/\eta, \tag{13}$$

$$a_{01}=0, \tag{14}$$

$$a_{20}=(\pi^2 k_{33}/4d)[k_s\cos^2\theta_1+\sin^2\theta_1-t(s+1)(r-s)\sin 2\theta_1/\eta^2], \tag{15}$$

$$a_{11}=0, \tag{16}$$

$$a_{02}=(\pi^2 k_{33}/4d)\{k_t\cos^2\theta_1+\sin^2\theta_1 - t\sin 2\theta_1[s+1+(1-2/\pi)(2r-l)/(l\cos^2\theta_1+2p\sin^2\theta_1)]/2\eta\}, \tag{17}$$

$$a_{30}=(2\pi k_{33}/9d)\{1{\cdot}5(1-k_s)\sin 2\theta_1 - 2t[(s+1)(r-s)/\eta^2][\cos 2\theta_1+(s+1)\sin^2 2\theta_1/\eta]\}, \tag{18}$$

$$a_{12}=(\pi k_{33}/3d)\{(1-k_s)\sin 2\theta_1-(2t/\eta)[(s+1)\cos 2\theta_1+(s+1)^2\sin^2 2\theta_1/2\eta + (2r-l)F(\theta_1)/(l\cos^2\theta_1+2p\sin^2\theta_1)]\}, \tag{19}$$

$$a_{21}=0, \tag{20}$$

$$a_{03}=0. \tag{21}$$

In these equations, the reduced quantities

$$k_s=k_{11}/k_{33},\quad k_t=k_{22}/k_{33},\quad s=\alpha_3/\alpha_2,\quad l=\alpha_4/\alpha_2,\quad p=(\alpha_4+\alpha_5-\alpha_2)/2\alpha_2$$

and

$$r=(\alpha_3+\alpha_4+\alpha_6)/2\alpha_2$$

have been introduced, and

$$\eta=r-(s+1)\sin^2\theta_1.$$

The reduced stress is defined by

$$t=\tau/\tau_0,$$

where

$$\tau_0=k_{33}\pi^2/d^2.$$

The function $F(\theta_1)$ in a_{12} has the form:

$$F(\theta_1)=\cos 2\theta_1-2\cos^2\theta_1/\pi+\sin^2\theta_1/2$$
$$+(\sin^2 2\theta_1/2)[3(s+1)/2\eta+(1/\pi+4/\pi-0{\cdot}5)(2p-l)/(l\cos^2\theta_1+2p\sin^2\theta_1)].$$

It is evident, that coefficient a_{10} vanishes for $\theta_1=\arctan\sqrt{s}$ and $\theta_1=-\arctan\sqrt{s}$. Together with $a_{01}=0$, this defines two critical points of G at $\xi=0$ and $\chi=0$. Analysis of the second derivative matrix

$$\mathbf{H}=\begin{bmatrix}\dfrac{\partial^2 G}{\partial\xi^2} & \dfrac{\partial^2 G}{\partial\xi\partial\chi}\\ \dfrac{\partial^2 G}{\partial\xi\partial\chi} & \dfrac{\partial^2 G}{\partial\chi^2}\end{bmatrix}, \tag{22}$$

which has a diagonal form in this problem, determines the degeneracy of both of them. Namely the value $\theta_1=\arctan\sqrt{s}$ gives the non-degenerate critical point (minimum), since $\det\mathbf{H}=a_{20}a_{02}$ remains always positive. On the other hand, the angle

$$\theta_1=-\theta_c=-\arctan\sqrt{s}, \tag{23}$$

gives the degenerate critical point, because $a_{20}a_{02}$ can vanish for some sets of other parameters. In particular, there exist two values of the critical stress

$$t_{c1}=(k_s+s)(s-r)/2\sqrt{s}(1+s), \tag{24}$$

$$t_{c2}=(k_t+s)(s-r)(2ps+l)/2\sqrt{s}(1+s)[r+ps-(2r-l)/\pi], \tag{25}$$

due to $a_{20}=0$ and $a_{02}=0$, respectively. Moreover, if

$$k_t=(k_s+s)[r+ps-(2r-l)/\pi]/(2ps+l)-s=k_c, \tag{26}$$

then they coincide:

$$t_{c1}=t_{c2}=t_c=(k_c+s)(s-r)(2ps+l)/2\sqrt{s}(1+s)[r+ps-(2r-l)/\pi]. \tag{27}$$

By application of rules given in [5], we can prove, that the Taylor series (12) may be limited to third order. Therefore, the function $G(\theta,\phi)$ is equivalent to its truncated expansion

$$G=a_{10}\xi+a_{20}\xi^2+a_{02}\chi^2+a_{12}\xi\chi^2+a_{30}\xi^3, \tag{28}$$

if only small deformations are considered and the parameters are not very different from their critical values given by equations (23), (26) and (27). By a suitable change of variables, this expression could be transformed into the standard form of the hyperbolic umbilic catastrophe [5]. It is, however, not necessary and later the untransformed form (28) will be used. The bifurcation set of the hyperbolic umbilic catastrophe divides the parameter space into four regions characterized by different numbers of extremes: (1) minimum, maximum and two saddle points; (2) minimum and one saddle point; (3) maximum and one saddle point; (4) no extremes. The continuous

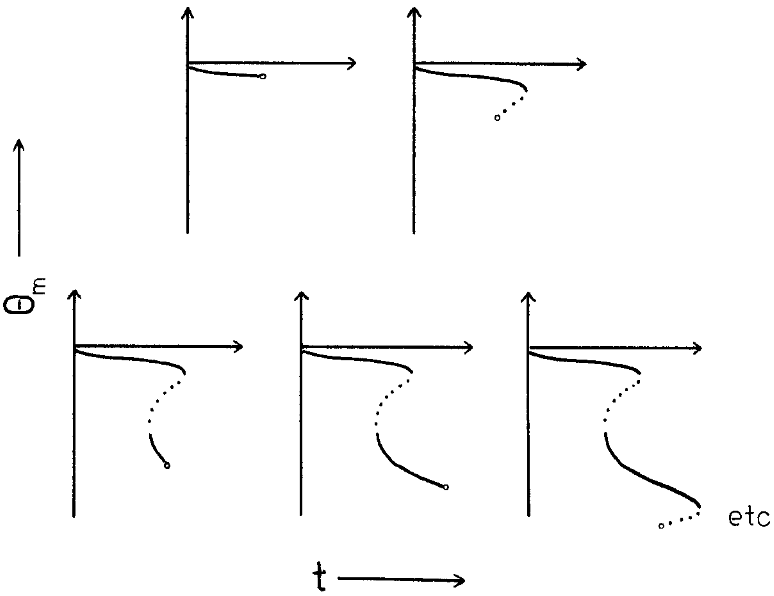

Figure 2. Several possibilities of the $\theta_m(t)$ dependence resulting from different relations between t_{c1} and t_{c2}. The circles on the ends of the lines denote coming out of the shear plane. Full line denotes minima and the dotted line denotes other extremes.

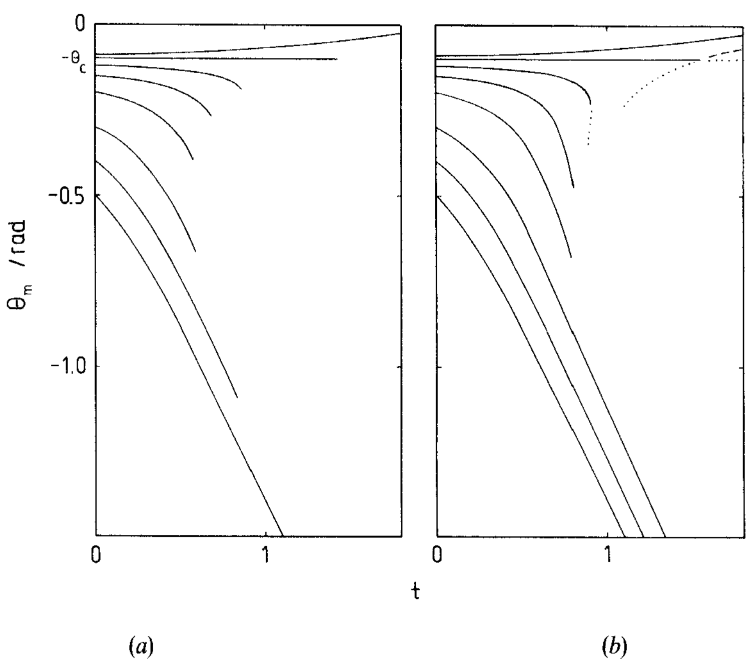

Figure 3. Examples of the $\theta_m(t)$ dependence for the flow-aligning nematics. $s=0{\cdot}01$, $r=-0{\cdot}3$, $l=-0{\cdot}9$, $p=-1{\cdot}31$, $k_s=1$; (a) $k_t=0{\cdot}4$; (b) $k_t=0{\cdot}6$. The coming out of the shear plane takes place at the end of each full line. Dashed line denotes unavailable minima.

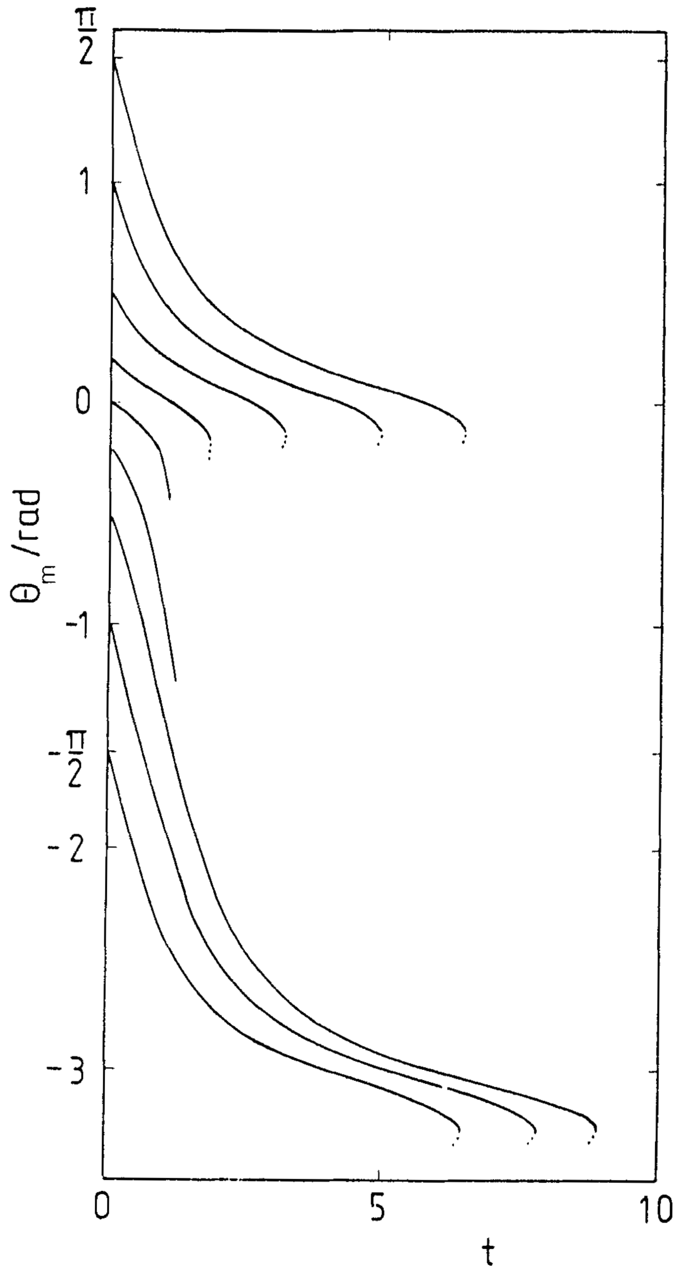

Figure 4. Examples of $\theta_m(t)$ dependence for the non-flow-aligning nematic. $s=-0{\cdot}053$, $r=-0{\cdot}396$, $l=-0{\cdot}99$, $p=-1{\cdot}343$, $k_s=1$, $k_t=0{\cdot}65$.

change of the shear stress is accompanied with the move of the corresponding point in the parameter space. The physically interesting effect takes place when this point passes for the first time across the boundary between regions (1) and (2) or (1) and (3). This is related to the loss of stability of the initial uniform director distribution: the minimum at ($\xi=0$, $\chi=0$) is replaced by the maximum. This corresponds to the lower of the threshold stresses t_{c1} and t_{c2}.

Two possible types of behaviour of the layer in the vicinity of the critical point can be distinguished. If $t_{c2} < t_{c1}$, i.e. if

$$k_t < (k_s + s)[r + ps - (2r - l)/\pi]/(2ps + l) - s, \tag{29}$$

then the director loses its stability in the plane of shear. This suggests a discontinuous transition to a deformed state ($\xi \neq 0$, $\chi \neq 0$), although this new equilibrium is not shown explicitly. If $t_{c1} < t_{c2}$, then two situations may take place at t_{c1}. The destabilization, mentioned previously, of the in-plane director distribution occurs for not too large k, as can be seen in figure 3. For sufficiently high k_t, the director does not deviate from its initial plane, and the state ($\xi \neq 0$, $\chi = 0$) is realized, as assumed in [3] and [4].

The behaviour of the system with θ_1 different from the critical value is described in the next section.

4. Arbitrary surface alignment angles and non-flow-aligning nematics

In the case of arbitrary surface alignment angles or of non-flow-aligning nematics, the critical point ($\xi = 0$, $\chi = 0$), which is related to the uniform initial orientation $\theta(z) = \theta_1$, disappears, since $a_{10} \neq 0$. Other critical points can be found, which are due to the deformed director field. The director distribution in the plane of shear, $\theta_0(z)$, can be obtained numerically; it is defined by the minimum of the function G. The small distorsions of this equilibrium state can be described by

$$\theta(z) = \theta_0(z) + \xi \cos(\pi z/d), \tag{30}$$

$$\phi(z) = \chi \cos(\pi z/d), \tag{31}$$

in analogy to equations (10) and (11). The coefficients of the Taylor expansion are now given by

$$a_{10} = (k\pi/d) \int [-\theta_z \sin(\pi z/d) + (\pi t/d)[(s\cos^2\theta_0 - \sin^2\theta_0)/\eta_0] \cos(\pi z/d)]\, dz, \tag{32}$$

$$a_{01} = 0, \tag{33}$$

$$a_{20} = (k\pi^2/4d)[1 - (2t/d)(s+1)(r-s) \int (\sin 2\theta_0/\eta_0^2) \cos^2(\pi z/d)\, dz], \tag{34}$$

$$a_{11} = 0, \tag{35}$$

$$\begin{aligned} a_{02} = (k\pi^2/4d) \int \{ &(2/d)(\sin^2\theta_0 + k_t \cos^2\theta_0) \sin^2(\pi z/d) \\ &- (2d/\pi^2)[1 + (1 - k_t)\sin^2\theta_0]\theta_z^2 \cos^2(\pi z/d) \\ &+ (2/\pi)(1 - k_t) \sin 2\theta_0 \theta_z \sin(\pi z/d) \cos(\pi z/d) \\ &- (t \sin 2\theta_0/\eta_0 d) \\ &\times [s + 1 + (1 - 2/\pi)(2r - l)/(l\cos^2\theta_0 + 2p\sin^2\theta_0)] \cos^2(\pi z/d)\}\, dz, \end{aligned} \tag{36}$$

$$a_{30} = -(k\pi^2/3d)t(s+1)(r-s) \int [\cos 2\theta_0/\eta_0^2 + (s+1)\sin^2 2\theta_0/\eta_0^3] \cos^3(\pi z/d)\, dz, \tag{37}$$

$$a_{12}=(k/d)\int\{(d/2)(k_t-1)\sin 2\theta_0\theta_z^2\cos^3(\pi z/d)$$
$$+\pi(1+\cos^2\theta_0+k_t\sin^2\theta_0-k_t)\theta_z\sin(\pi z/d)\cos^2(\pi z/d)$$
$$-(\pi^2/2\eta_0 d)t[(s+1)\cos 2\theta_0+(s+1)^2\sin^2 2\theta_0/2\eta_0$$
$$+(2r-l)F(\theta_0)/(l\cos^2\theta_0+2p\sin^2\theta_0)]\cos^3(\pi z/d)\}\,dz, \quad (38)$$

$$a_{21}=0, \quad (39)$$

$$a_{03}=0, \quad (40)$$

where

$$\theta_z=\partial\theta_0(z)/\partial z, \quad \eta_0=r-(s+1)\sin^2\theta_0(z),$$

and integration is performed from $-d/2$ to $d/2$. The function $F(\theta_0)$ in a_{12} has the form

$$F(\theta_0)=\cos 2\theta_0-2\cos^2\theta_0/\pi+\sin^2\theta_0/2$$
$$+(\sin^2 2\theta_0/2)[3(s+1)/2\eta+(1/\pi+4/\pi-0{\cdot}5)(2p-l)/(l\cos^2\theta_0+2p\sin^2\theta_0)].$$

To simplify the computations, the equality $k_{11}=k_{33}=k$ is assumed, this enables us to use the relation [6]

$$\frac{\partial\theta_0(z)}{\partial z}=\pi\sqrt{(2t)}\left\{\theta_0-\theta_m+\frac{r-s}{\sqrt{(r-p)}}\left[\arctan\left(\tan\theta_0\sqrt{\frac{r}{p}}\right)-\arctan\left(\tan\theta_m\sqrt{\frac{r}{p}}\right)\right]\right\}^{1/2},$$

where θ_m is the midplane director orientation angle. All of the considerations made in the preceding section are valid. In consequence the hyperbolic umbilic catastrophe is also suitable for description of this generalized case. Since the deformation starts smoothly from $t=0$, the critical stress t_{c1} does not now play the role of any threshold. There can be zero or two t_{c1} values in the flow-aligning nematics and an unlimited number if $s<0$. They correspond to jumps between the deformed states which differ significantly in their elastic energy. For non-flow-aligning nematics, this effect is known as tumbling. The critical field t_{c2} corresponds to coming out of the shear plane. The behaviour of the system is determined by the relation between t_{c1} and the lowest value of t_{c2},. The possibilities are shown in figure 2, where θ_m is plotted schematically against t, some of them can be found in flow-aligning materials.

The results of detailed calculations are presented in figures 3 and 4. They illustrate the role of θ_1 and k_t for the behaviour of the layer. In the flow-aligning materials, coming out of the shear plane can occur for a limited range of θ_1 values. This effect is possible also for k_t which do not satisfy the inequality (29), however the range of θ_1 is especially narrow for high values of k_t. If k_t is too high, then the director remains in the plane of shear at any θ_1. There is no coming out for $0\leqslant\theta_1\leqslant\pi/2$, and so for planar or homeotropic alignment also. If $s<0$, then coming out occurs for any θ_1, but for especially high k_t, very strong deformation is required.

5. Concluding remarks

Summarizing, the stability of the director in the plane of shear during the simple shear flow was studied by use of a method based on catastrophe theory. It was found, that the effect of coming out of the shear plane occurred not only for the non-flow-aligning nematics, but for the flow-aligning materials as well. The results have a qualitative character, they can serve as a useful stimulous for accurate numerical investigations.

The umbilic catastrophe, which was applied here, gives no information about the deformed out-of-the-shear-plane state. This is a consequence of low order of the power expansion, which is sufficient only for a proper determination of the critical point and its close neighbourhood. In all the cases of coming out, the equilibrium state, in which the director lies in the shear plane, disappears abruptly. This suggests a discontinuous transition with hysteresis to a deformed state ($\xi \neq 0$, $\chi \neq 0$). In the present work, the particular case is considered, in which the director is initially aligned parallel to the plane of shear. This leads to the incomplete (non-universal) form of the catastrophe [5]. The abrupt disappearance of the undeformed state results from this limitation. In the general case, when the critical alignment is not parallel to the shear plane, the director may come out smoothly starting from $t=0$. Such a behaviour may be expected from the analogy with other transitions, for example, in an electric field [7].

Several approximations were adopted during the calculations and they are justified by the qualitative character of the method used. The threshold values of the shear stress are given by equations (24) and (25) with an accuracy resulting from the unknown role of α_1 which was neglected. The $\theta_m(t)$ dependence is obtained with the additional approximation $k_{11}=k_{33}$.

The role of the geometric and material parameters is evident. If $s>0$, then the small values of k_t and moderate surface tilts are conducive to coming out of the shear plane. In agreement with earlier experiments and theoretical considerations, this effect occurs neither for homeotropic nor for planar alignment. In the case of non-flow-aligning nematics, the behaviour of the layer depends on the relation between t_{c1} (if it exists) and t_{c2}. This relation decides which effect takes place: tumbling or coming out of the shear plane. The latter effect seems to be unavoidable, although for high k_t, rather strong deformations with large $|\theta_m|$ are required. The coming out of the shear plane occurs only if θ_m takes negative values. These statements are consistent with results obtained by Zuniga and Leslie [1, 2]. The results described in [3, 4] are valid for materials with sufficiently high k_t, since no possibility of coming out was taken into account there.

Appendix

Each component of the function g gives rise to a_{ij} coefficients and can be expanded separately in a Taylor series. The expansion of g_{elastic} and its integration over z is straightforward. The calculations due to the viscous parts are more laborious, but some relations can be found, which simplify the procedure.

The viscous parts of the function g can be expressed as (see equation (6))

$$g_{\text{viscous}} = -\int_0^\theta \Gamma_x\Big|_{\phi=0} d\theta - \int_0^\phi \Gamma_{yz}\Big|_{\theta=\text{const}} d\phi. \tag{A 1}$$

The function

$$\int_0^\theta \Gamma_x\Big|_{\phi=0} d\theta,$$

does not depend on ϕ and so its derivatives with respect to χ vanish, and the Taylor series contains only the derivatives with respect to ξ. They can be obtained easily by use of Γ_x. Since the zero-degree term is not important, the integration is not necessary. The same argument applies to the function

$$\int_0^\phi \Gamma_{yz}\Big|_{\theta=\text{const}} d\phi,$$

for any θ, it is equal to zero at $\phi=0$. It means, that its derivatives with respect to ξ vanish. However there remain $\partial\Gamma_{yz}/\partial\chi$ and its higher derivatives with respect to ξ and χ, and they give rise to the coefficients a_{ij}.

The components of the viscous torques are:

$$\Gamma_x = -u\cos^2\phi(\alpha_3\cos^2\theta-\alpha_2\sin^2\theta)-w\alpha_3\sin\phi\cos\phi\cos\theta, \tag{A 2}$$

$$\Gamma_y = u\alpha_3\sin\phi\cos\phi\cos\theta+w(\alpha_3\sin^2\phi-\alpha_2\cos^2\phi\sin^2\theta), \tag{A 3}$$

$$\Gamma_z = -u\alpha_2\sin\phi\cos\phi\sin\theta+w\alpha_2\cos^2\phi\sin\theta\cos\theta, \tag{A 4}$$

where $u=\partial v_y/\partial z$ and $w=\partial v_x/\partial z$ are given by the Navier–Stokes equations:

$$2\tau=[\alpha_4+(\alpha_5-\alpha_2)\cos^2\phi\sin^2\theta+(\alpha_3+\alpha_6)\cos^2\phi\cos^2\theta]u + (\alpha_3+\alpha_6)\sin\phi\cos\phi\cos\theta w, \tag{A 5}$$

$$2\sigma=(\alpha_3+\alpha_6)\sin\phi\cos\phi\cos\theta u + [\alpha_4+(\alpha_5-\alpha_2)\cos^2\phi\sin^2\theta+(\alpha_3+\alpha_6)\sin^2\phi]w, \tag{A 6}$$

in which α_1 is neglected and σ denotes the transverse shear stress. From this set of equations, u and w can be obtained, and then used to calculate Γ_{yz}. For compact notation, equations (A 5) and (A 6) are rewritten as

$$2\tau=Pu+Qw, \tag{A 7}$$

$$2\sigma=Qu+Rw. \tag{A 8}$$

Then

$$\Gamma_{yz}=Ku+Jw=A\tau+B\sigma, \tag{A 9}$$

where

$$K=(\alpha_2+\alpha_3)\sin\phi\cos\phi\sin\theta\cos\theta, \tag{A 10}$$

$$J=\sin\theta(\alpha_3\sin^2\phi-\alpha_2\cos^2\phi), \tag{A 11}$$

$$A=2(KR-JQ)/\Delta, \tag{A 12}$$

$$B=2(JP-KQ)/\Delta, \tag{A 13}$$

$$\Delta=PR-Q^2. \tag{A 14}$$

The angles θ and ϕ are given by equations (10) and (11) or (30) and (31).

The transverse shear stress σ is induced by the external shear stress τ and results only if the director deviates from the plane of shear. Its value results from the condition related to the no-slip assumption for transverse flow

$$\int_{-d/2}^{d/2} w\,dz=0, \tag{A 15}$$

which gives

$$\sigma=\tau\frac{\int_{-d/2}^{d/2}(Q/\Delta)\,dz}{\int_{-d/2}^{d/2}(P/\Delta)\,dz}. \tag{A 16}$$

The integrals in this equation are calculated by use of the expansion of the integrands in a power series of ξ and χ. The expressions which include σ appear in the a_{ij} coefficients and are taken, in their final form, at the critical point $\xi=0$, $\chi=0$. Therefore only the first term of the integrated series gives rise to them:

$$\int_{-d/2}^{d/2} (Q/\Delta)\,dz\bigg|_{\substack{\xi=0\\ \chi=0}} = (Q/\Delta)\bigg|_{\substack{\xi=0\\ \chi=0}} \int_{-d/2}^{d/2} dz = 0, \tag{A 17}$$

$$\int_{-d/2}^{d/2} (P/\Delta)\,dz\bigg|_{\substack{\xi=0\\ \chi=0}} = (P/\Delta)\bigg|_{\substack{\xi=0\\ \chi=0}} \int_{-d/2}^{d/2} dz = d/R. \tag{A 18}$$

This also applies to the derivatives of σ with respect to ξ and χ, which are present in the expressions for the derivatives of Γ_{yz}. For instance

$$\frac{\partial\sigma}{\partial\xi} = \tau\left[\frac{\dfrac{\partial}{\partial\xi}\displaystyle\int (Q/\Delta)\,dz}{\displaystyle\int (P/\Delta)\,dz} - \frac{\displaystyle\int (Q/\Delta)\,dz \frac{\partial}{\partial\xi}\int (P/\Delta)\,dz}{\left(\displaystyle\int (P/\Delta)\,dz\right)^2}\right], \tag{A 19}$$

which leads to

$$\frac{\partial\sigma}{\partial\xi}\bigg|_{\substack{\xi=0\\ \chi=0}} = \tau\frac{\dfrac{\partial Q}{\partial\theta}\bigg|_{0,0}\displaystyle\int \cos(\pi z/d)\,dz}{P|_{0,0}\,d} = 0. \tag{A 20}$$

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