Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

Analysis of shear flow alignment of nematic liquid crystals at low shear stress based on catastrophe theory

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To cite this Article Derfel, G.(1989) 'Analysis of shear flow alignment of nematic liquid crystals at low shear stress based on catastrophe theory', Liquid Crystals, 6: 6, 709 — 716
To link to this Article: DOI: 10.1080/02678298908029113
URL: http://dx.doi.org/10.1080/02678298908029113

LIQUID CRYSTALS, 1989, VOL. 6, NO. 6, 709–716

Analysis of shear flow alignment of nematic liquid crystals at low shear stress based on catastrophe theory

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(*Received 7 March 1989; accepted 24 July 1989*)

The low stress shear flow alignment of a nematic liquid crystal in the presence of strong anchoring at the boundaries is analysed. Layers with pretilted director orientation are taken into account. Two kinds of symmetric deformations are assumed. They differ in the director distribution in the vicinity of the boundaries. The analysis is carried out using an expansion of the free energy of the layer in powers of the maximum deformation angle. The results have qualitative character. The condition for the threshold behaviour and the stability of the solutions are discussed. The deformation may develop continuously or discontinuously. The transition between two kinds of deformation is predicted. The facts already known are confirmed and supplemented.

1. Introduction

The influence of flow upon the alignment of nematic liquid crystals is well known. It has been applied in numerous viscometric experiments [1–3], and explained in terms of continuum theory [4–6]. In this paper, the simple shear flow of a nematic is considered in the presence of elastic effects due to strong anchoring of the director on the boundary plates. The director orientation in the mid-plane of the layer is sought and the onset of flow orientation is analysed. The analysis is restricted to steady state deformations of the nematic for which $\alpha_3/\alpha_2 > 0$. The variety of the possible solutions, which stems from the competition between solid surfaces and flow, is investigated by means of method applied in a previous paper [7] to field effects in nematics. It is based on an analysis of a truncated Taylor expansion of the free energy of the system. The order of the truncated series is determined by application of theorems from catastrophe theory.

Catastrophe theory predicts the number and kind of critical points of the function considered i.e. the points at which the first derivative vanished. The behaviour of the system depends on the degeneracy of the critical point, i.e. the number of the sucessive higher derivatives which are zero at this point. The most interesting phenomena occur in the vicinity of the degenerate, critical point. Thresholds or discontinuities are the characteristic features of this behaviour. In this paper, the so-called cusp catastrophe is used, its properties were briefly described earlier [7]. In §2, this catastrophe is applied to the problem of shear flow alignment, the results are presented in §3 and discussed in §4.

2. Method

The geometry of the system considered is shown in figure 1. The nematic is confined between two infinite parallel plates a distance d apart. It is characterized by Leslie viscosity coefficients α_2 and α_3, Męsowicz viscosity coefficients η_2 and elastic

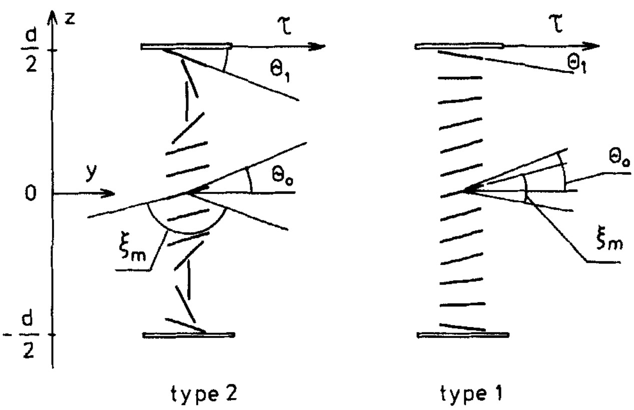

Figure 1. The definition of the angles describing the geometry of the sheared nematic layer for two types of deformation.

constants k_{11} and k_{33}. The analysis is restricted to the case $\alpha_3/\alpha_2 > 0$. The director is oriented on both boundaries in one direction with a preliminary tilt θ_1. (The angles are counted positive for anticlockwise rotation.) Under the action of the constant shear stress τ, one of the plates moves with respect to the other and the director field is deformed. It can be assumed that the director remains in the shear plane zy; its components are $n_x = 0$, $n_y = \cos\theta(z)$, $n_z = \sin\theta(z)$, where $\theta(z) = \theta_1 + \xi(z)$. The symmetrical shape of the $\xi(z)$ function proposed by Leslie [4] is assumed. For small deformations, the function $\xi(z)$ can be approximated by the first term of its Fourier expansion:

$$\xi(z) = \xi_m \cos(\pi z/d). \tag{1}$$

The torque exerted on the director consists of the elastic part and the viscous part. The distortion of the director field is connected with the free energy density

$$\mathscr{E} = \mathscr{E}_{\text{elastic}} + \mathscr{E}_{\text{viscous}}; \tag{2}$$

here $\mathscr{E}_{\text{elastic}}$ is given by

$$\mathscr{E}_{\text{elastic}} = (1/2)k_{33}[1 - K\cos^2\theta(z)](d\theta/dz)^2 \tag{3}$$

where $K = 1 - k_{11}/k_{33}$. $\mathscr{E}_{\text{viscous}}$ can be obtained by integration of the viscous torque per unit volume

$$\mathscr{E}_{\text{viscous}} = \int \frac{\alpha_3\cos^2\theta - \alpha_2\sin^2\theta}{\eta_2 - (\alpha_2 + \alpha_3)\sin^2\theta}\,\tau\, d\theta, \tag{4}$$

$$= \tau\left[\theta - \frac{\eta_2 - \alpha_3}{\sqrt{(\eta_1\eta_2)}}\arctan(\operatorname{tg}\theta(\eta_1/\eta_2))\right], \tag{5}$$

where $\eta_1 = \eta_2 - \alpha_2 - \alpha_3$ according to Parodi relation, and the small contribution of the α_1 coefficient has been neglected. Using equations (1) to (5) we can calculate the free energy per unit area of the layer, G. For this purpose the free energy density is first expanded in a Taylor series of ξ_m in the vicinity of $\xi_m = 0$, and then integrated. The resulting expression has the form

$$G = a_0 + a_1\xi_m + a_2\xi_m^2 + a_3\xi_m^3 + a_4\xi_m^4 + O(5). \tag{6}$$

The term a_0 is unimportant, as it can be removed by a suitable choice of the energy zero. The coefficients $a_1 \ldots a_4$ are given by

$$a_1 = \frac{2\pi k_{33}}{d}(t/\eta)(s\cos^2\theta_1 - \sin^2\theta_1), \tag{7}$$

$$a_2 = \frac{\pi^2 k_{33}}{4d}\left\{1 - K\cos^2\theta_1 - t\frac{(s+1)(r-s)\sin 2\theta_1}{\eta^2}\right\}, \tag{8}$$

$$a_3 = \frac{2\pi k_{33}}{9d}\left\{1{\cdot}5K\sin 2\theta_1 - 2t\frac{(s+1)(r-s)}{\eta^2}\left[\cos 2\theta_1 + \frac{(s+1)\sin^2 2\theta_1}{\eta}\right]\right\}, \tag{9}$$

$$a_4 = \frac{\pi^2 k_{33}}{16d}\left\{K\cos 2\theta_1 + t\frac{(s+1)(r-s)}{\eta^2}\sin 2\theta_1 \times\left[1 - \frac{3(s+1)\cos\theta_1}{\eta} - \frac{1{\cdot}5(s+1)^2\sin^2 2\theta_1}{\eta^2}\right]\right\}, \tag{10}$$

where the reduced quantities $s = \alpha_3/\alpha_2$ and $r = \eta_2/\alpha_2$, and $\eta = r - (s+1)\sin^2\theta_1$ have been introduced. The reduced shear stress t is defined by

$$t = \tau/\tau_0, \tag{11}$$

where $\tau_0 = k_{33}\pi^2/d^2$. The critical point at $\xi_m = 0$ (for the non-trivial case of $s > 0$ and $t \neq 0$) obtains if $\mathrm{tg}\,\theta_1 = \pm\sqrt{s}$. This point can be, at most, twofold degenerate, as a_4 is the first coefficient which cannot be lead to zero by any choice of material parameters found for real liquid crystals. According to the theorems of catastrophe theory, the expansion of the energy G can be limited to fourth degree and the system is qualitatively described by the cusp catastrophe. The behaviour of the director in the layer can be analysed by a variation of the parameters. Here, the reduced shear stress is varied, whereas the other parameters are fixed. The positive values of t are considered and since the surface tilt angle covers the range from $-\pi/2$ to $\pi/2$, all possible situations are taken into account. In particular $a_2 = 0$ if t takes a critical value

$$t_c = \frac{(1+s-K)(s-r)}{2\sqrt{s}(1+s)}. \tag{12}$$

For typical material constants: $s = 0{\cdot}01$, $r = -0{\cdot}2$, $K = 0{\cdot}3$, $k_{33} = 10^{-11}N$ and $d = 10^{-5}$ m, the absolute value of t_c is about $0{\cdot}7\,\mathrm{N/m^2}$.

The extremes of G are calculated from the minimalization condition for some distinct cases. The existence of extremes and their disposition is predicted properly in the vicinity of the critical points, whereas the numerical values of ξ_m are only approximate.

3. Results

3.1. *Threshold behaviour*

The critical points can be achieved if $a_1 = 0$; for $t \neq 0$, this is possible if $\mathrm{tg}\,\theta_1 = +\sqrt{s}$ or if $\mathrm{tg}\,\theta_1 = -\sqrt{s}$. In the former cases, a_2 remains different from zero for any positive t. It means that there is always an energy minimum at $\xi_m = 0$. Therefore the orientation at the angle $\theta_1 = \mathrm{artcan}\sqrt{s}$, denoted by θ_0, is stable and uniform throughout the sample. In the latter case, when $\theta_1 = -\theta_0$, there exists a threshold stress t_c given by equation (12). Above this value deformation occurs, usually discontinuously. Two types of deformation can be distinguished and they are shown schematically in figure 1. On the basis of the torque equation for $t \to \infty$, we can relate type 1 to the high stress flow alignment angle θ_0 and type 2 to the angle $\theta_0 - \pi$. If a_3 is negative at the threshold, which can be expressed by

$$K < \frac{r + 3s + (4 - r)s^2 + s^3}{r + (3 + 2r)s - 2s^2}, \tag{13}$$

then the deformation angle is positive, (see figure 3c); this corresponds to type 1. In the opposite case, type 2 is realized (see figure 3(*a*)). If $a_3 = 0$, both types of deformation are equally probable and the deformation develops continuously, as only positive values of a_4 occur at the threshold for real nematics (see figure 3(*b*)).

3.2. *Thresholdless behaviour*

If $\mathrm{tg}^2\,\theta_1 \neq s$, the coefficient a_1 vanishes only for $t = 0$ and this critical point is non-degenerate. Therefore the behaviour of the system in the vicinity of $t = 0$ is properly described by the Taylor expansion of G truncated at the quadratic term. From the minimalization condition, we obtain the expression

$$\xi_m = -a_1/2a_2 \tag{14}$$

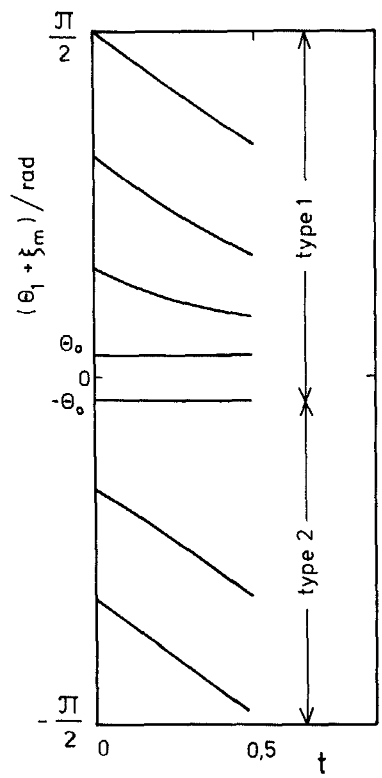

Figure 2. The initial behaviour of the orientation angle $\theta_1 + \xi_m$ calculated for different surface tilt angles θ_1, $k_{33}/k_{11} = 1{\cdot}2$, $s = 0{\cdot}01$, $r = -0{\cdot}2$.

and its derivative with respect to t at $t = 0$ is equal to

$$\left.\frac{d\xi_m}{dt}\right|_{t=0} = \frac{4(s\cos^2\theta_1 - \sin^2\theta_1)}{\pi(1 - K\cos^2\theta_1)[(s+1)\sin^2\theta_1 - r]}; \tag{15}$$

it is positive if

$$-\arctan\sqrt{s} < \theta_1 < \arctan\sqrt{s}. \tag{16}$$

The deformation angle increases according to deformation of type 1. In the opposite case, taking place if

$$\arctan\sqrt{s} < -\theta_1 \quad \text{or} \quad \arctan\sqrt{s} > \theta_1, \tag{17}$$

the deformation angle is negative. This corresponds to type 1 for $\theta_0 < \theta_1 < \pi/2$ and to type 2 for $-\pi/2 < \theta_1 < -\theta_0$.

These results are gathered in figures 2 and 3. The curves approximate well to the real $\xi_m(t)$ functions, the closer to the critical point are the parameters of the system. Figure 2 shows the initial tendencies of the $\xi_m(t)$ dependence for the whole range of θ_1; they are similar for any sign of a_3. The details of the behaviour in the vicinity of the critical point are shown in figure 3.

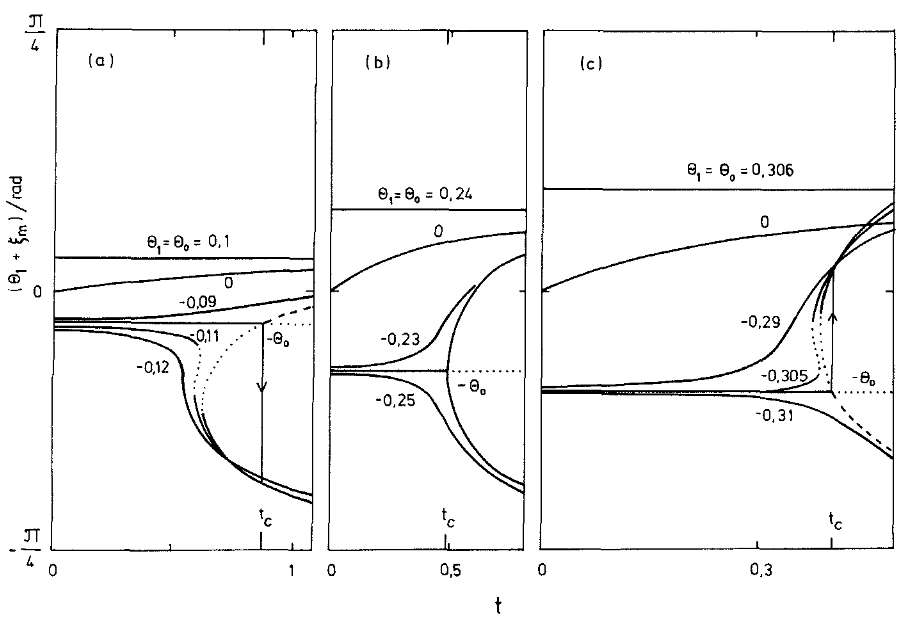

Figure 3. The director orientation $\theta_1 + \xi_m$ as a function of the reduced stress t. $r = -0{\cdot}2$; (*a*) $s = 0{\cdot}01$, $k_{33}/k_{11} = 1{\cdot}2$, $a_3 > 0$; (*b*) $s = 0{\cdot}06$, $k_{33}/k_{11} = 1{\cdot}1$, $a_3 = 0$; (*c*) $s = 0{\cdot}1$, $k_{33}/k_{11} = 1{\cdot}2$, $a_3 < 0$. The values of θ_1 are indicated. Full line—minima, dotted line—maxima, dashed line—unavailable minima. The non-essential solutions are omitted for clarity.

3.3. *Transition between two types of deformation*

It is evident from figure 2, that the type of deformation results from the relation between θ_1 and $-\theta_0 = -\arctan\sqrt{s}$. In typical experiments on shear flow alignment, the homeotropic or planar surface orientation was assured and sufficiently high stress was applied to the layer ([3], [8]). In these situations, type 1 of deformation is realized for arbitrary values of the material constants. The orientation in the middle of the layer is determined by θ_0 and varies smoothly with temperature. There are however such values of θ_1, which may be taken by $-\arctan\sqrt{s}$ during variation of temperature. A rapid change of the director distribution may take place in such a case, due to the transition from one type of deformation to another. The occurrence of this effect can be investigated by an analysis of the trajectories on the control plane (see [7]). If the trajectory intersects the bifurcation set twice, the discontinuity takes place in the second point of the intersection. Figure 4 shows some examples of the trajectories corresponding to the change of stress at constant temperature (lines AE and BF), and to the change of temperature at constant stress (lines CD and EF). The parameters for 4-methoxybenzylidene-4′-n-butylaniline (MBBA) taken from [9] and [10], and the surface tilt $\theta_1 = -0{\cdot}18$ are used. The transition takes place if the path BDC or similar is realized. Therefore the deformation should be induced at high temperature and then the layer should be cooled at moderate stress. We may suppose that the rapid change of the director profile is accompanied by a discontinuity in the temperature dependence of the apparent viscosity. Other transitions of this kind are possible if only the trajectory leaves the area between the branches of the bifurcation set.

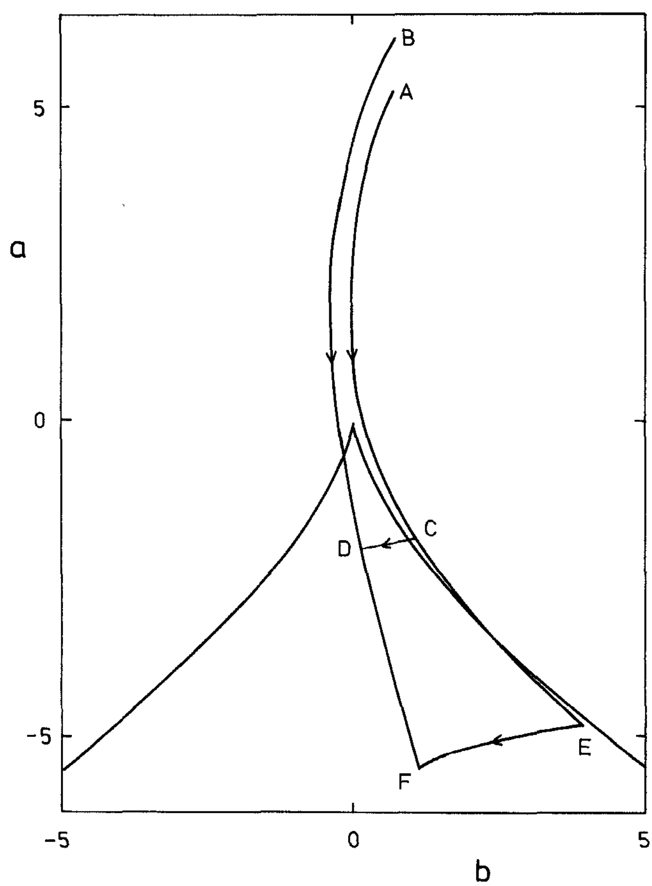

Figure 4. The trajectories corresponding to the change of stress (AE, $T = 20°C$, and BF, $T = 42°C$), and to the change of temperature (CD, $t = 3$, and EF, $t = 16$) for MBBA, $\theta_1 = -0{\cdot}18$. The arrows indicate the increase of the quantity varied.

4. Discussion

The results obtained in the previous section provide a view of the development of flow alignment in nematic liquid crystals. They agree with results found by Currie and MacSithigh in [5] and [6] and extend some of their statements. The calculations were performed without restrictions on the values of the elastic constants. This gives a more detailed value for the threshold (see equation (12)). Two types of deformations, denoted by 1 and 2, are distinguished in a different manner to that in [6]. It is shown, that, depending on the material constants of a nematic, the sign of $a_3(t_c)$ and therefore the type of deformation is determined. Typical parameters, for instance those measured for MBBA, correspond to the behaviour shown in figure 3a. Currie and MacSithigh [6] pointed out that some symmetrical distributions of the director lose their stability. This is concerned with the undeformed state of the layer aligned at an angle $-\theta_0$, which became unstable above a critical stress, and the layer with surface tilt θ_1 slightly below $-\theta_0$. It follows from considerations of §3, that discontinuous transitions to the stable deformed configurations occur in such situations. The jumps take place at $t = t_c$ if $\theta_1 = -\theta_0$, and at $t < t_c$ if θ_1 is close to $-\theta_0$, the latter case is realized not only for $\theta_1 < -\theta_0$ if $a_3 > 0$, but also for $\theta_1 > -\theta_0$ if $a_3 < 0$.

Two significant approximations were employed for the calculations presented in this paper. The deformation was described by only its first Fourier component and the free energy power series was truncated at fourth degree. Approximations of this type are an inherent feature of the method applied. They allow us to recognize the nature of the critical point. Hence the correct picture of the behaviour of the system in the vicinity of this point can be obtained. The limitations placed on the results because of the approximations relate to the numerical values, not to the qualitative features. The parameters which determine the critical point are strictly known; other numerical values are only approximate. The data in figures 2 and 3 have only illustrative worth. In addition the range of θ_1, for which the discontinuities take place, cannot be strictly determined. However the tendency of the $\xi_m(t)$ dependence is presented properly, and allows us to predict the type of solution. This also concerns the transitions described in §3.3. The detailed values of the stress and the temperature, at which the jump occurs, are not obtainable. The results can be compared with those found from the numerical solution of the Euler–Lagrange equation [11]. The numerically calculated director distribution is sinusoidal to within an accuracy of several percent only if the deformation is far from saturation. The shape of the $\xi_m(t)$ dependence is the same as in figure 3, but the proportions between various parts of the curves may be different. In addition a rapid change in the apparent viscosity due to the transition between two types of deformation is found. Thus the qualitative features of the behaviour obtained in the approach presented are confirmed. For the class of nematic liquid crystals characterized by $s < 0$, the non-degenerate critical point takes place at $t = 0$. Only the low stress deformations are recognizable. The angle ξ_m takes negative values for any θ_1, in agreement with [12].

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