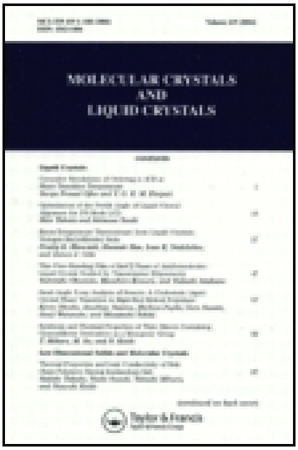

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

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Version of record first published: 24 Sep 2006

Mol. Cryst. Liq. Cryst., 1997, Vol. 292, pp. 113–122
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Flow Alignment in Biaxial and Discotic Nematics

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Continuum theory for nematic liquid crystals predicts two distinct types of flow alignment, one that observed in thermotropic rod-like nematics, and the second not so far observed but thought to be relevant to discotic nematics. This paper examines this latter possibility by considering recent flow alignment predictions for biaxial nematics, particularly for such materials where the molecular structure is close to discotic, and obtains results that support this claim. In addition it shows that in the disc-like limit biaxial theory reduces to that for a uniaxial nematic with viscosities consistent with this conjecture.

Keywords: Nematics; uniaxial nematic; continuum theory; biaxial nematic; flow alignment; discotic nematic

1. INTRODUCTION

Flow alignment in the theory for uniaxial nematics due to Ericksen [1] and Leslie [2] depends upon the values of two viscosity coefficients α_2 and α_3. When both are negative the theory predicts [3] alignment within the plane of shear at a relatively small acute angle to the streamlines in the positive direction of the shear gradient, this in agreement with observed behaviour. A second prediction, when α_2 and α_3 are both positive, is of flow alignment within the plane of shear at a relatively large acute angle to the streamlines in the negative direction of the shear gradient. This latter prediction is largely overlooked since positive values for both of these viscosities are not found for thermotropic nematics. However, motivated

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by some microscopic calculations of flow alignment by Forster [4] and Volovic [5], Carlsson [6, 7] suggests that this latter prediction may be relevant for discotic nematics, and here our aim is to present some support for this viewpoint.

Following the discovery by Yu and Saupe [8] of a lyotropic biaxial nematic, a number of authors have formulated phenomenological theories for biaxial nematics with Saupe [9], Govers and Vertogen [10], Chauré [11] and Leslie, Laverty and Carlsson [12] all obtaining essentially the same continuum theory from different standpoints. In a subsequent paper Leslie [13] discusses flow alignment in such theory and achieves a rather complete description, showing that whatever the values of the various viscous coefficients there is at most one predicted flow alignment configuration based on simple stability arguments. Naturally it seems reasonable to use his results in order to see what they predict for flow alignment of disc-like nematics, and whether or not they offer support for Carlsson's conjecture.

One can of course consider a biaxial nematic as a liquid in which the fluid elements have an elliptic platelet structure as opposed to the uniaxial rod-like description. Indeed biaxial nematics can be thought of as a progression from rod-like through elliptic platelets to disc-like, uniaxial and discotic therefore forming two extremes or limits of biaxial behaviour. Here we consider both limits and show first that predictions in the uniaxial limit are consistent with uniaxial theory. In the second limit with reasonable assumptions concerning the viscous coefficients our conclusions support Carlsson's prediction. This is further supported in a final section by showing that biaxial theory in the discotic limit reduces to a uniaxial theory fully consistent with his predictions.

Throughout the paper we employ Cartesian tensor notation, so that a comma preceding a suffix denotes partial differentiation with respect to the corresponding spatial coordinate, and repeated suffices are subject to the summation convention.

2. CONTINUUM THEORY FOR NEMATICS

Continuum theory for biaxial nematics employs two orthonormal vectors or directors, **n** and **m**, which clearly satisfy

$$n_i n_i = m_i m_i = 1, \quad n_i m_i = 0, \tag{2.1}$$

and commonly assumes incompressibility so that the velocity vector $\mathbf{v}$ is constrained by

$$v_{i,i}=0. \tag{2.2}$$

The balance laws representing conservation of linear and angular momentum are

$$\rho\frac{dv_i}{dt}=\rho F_i+t_{ij,j}, \quad \rho K_i+e_{ijk}t_{kj}+\ell_{ij,j}=0, \tag{2.3}$$

where ρ denotes constant density, $\mathbf{F}$ and $\mathbf{K}$ body force and moment per unit mass, and $\mathbf{t}$ and ℓ stress and couple stress tensors, respectively. The time derivative is of course the material time derivative.

The stress and couple stress in (2.3) are given by

$$t_{ij}=-p\delta_{ij}-\frac{\partial W}{\partial n_{k,j}}n_{k,i}-\frac{\partial W}{\partial m_{k,j}}m_{k,i}+\tilde{t}_{ij},$$

$$\ell_{ij}=e_{ipq}\left(n_p\frac{\partial W}{\partial n_{q,j}}+m_p\frac{\partial W}{\partial m_{q,j}}\right), \tag{2.4}$$

where p is an arbitrary pressure arising from the assumed incompressibility, and W is an elastic energy dependent upon the directors and their spatial gradients, quadratic in the latter, but its explicit form is not given, not being required in what follows. The tensors δ_{ij} and e_{ijk} are the Kronecker delta and the alternator, respectively. The dynamic or viscous stress $\tilde{\mathbf{t}}$ takes the form

$$\begin{aligned}\tilde{t}_{ij}&=\alpha_1 n_k n_p A_{kp} n_i n_j+\alpha_2 N_i n_j+\alpha_3 N_j n_i+\alpha_4 A_{ij}+\alpha_5 A_{ik} n_k n_j\\&+\alpha_6 A_{jk} n_k n_i+\beta_1 m_k m_p A_{kp} m_i m_j+\beta_2 M_i m_j+\beta_3 M_j m_i\\&+\beta_5 A_{ik} m_k m_j+\beta_6 A_{jk} m_k m_i+N_p m_p(\mu_1 m_i n_j+\mu_2 m_j n_i)\\&+n_k m_p A_{kp}(\mu_3 m_i n_j+\mu_4 m_j n_i),\end{aligned} \tag{2.5}$$

where

$$N_i=\frac{d}{dt}n_i-W_{ip}n_p, \quad M_i=\frac{d}{dt}m_i-W_{ip}m_p, \tag{2.6}$$

$$2A_{ij} = v_{i,j} + v_{j,i}, \quad 2W_{ij} = v_{i,j} - v_{j,i},$$

and the coefficients are simply constants.

For many purposes it is convenient to express the axial vector arising from the asymmetric part of the viscous stress in terms of two vectors $\mathbf{g}^n$ and $\mathbf{g}^m$ as follows

$$e_{ijk}\tilde{t}_{kj} = e_{ijk}(n_j\tilde{g}_k^n + m_j\tilde{g}_k^m), \tag{2.7}$$

and thus

$$\tilde{g}_i^n = -(\gamma_1 N_i + \gamma_2 A_{ip}n_p + \gamma_3 N_p m_p m_i + \gamma_4 n_k m_p A_{kp} m_i), \tag{2.8}$$

$$\tilde{g}_i^m = -(\lambda_1 M_i + \lambda_2 A_{ip} m_p),$$

where

$$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5, \quad \gamma_3 = \mu_2 - \mu_1, \quad \gamma_4 = \mu_4 - \mu_3,$$

$$\lambda_1 = \beta_3 - \beta_2, \quad \lambda_2 = \beta_6 - \beta_5. \tag{2.9}$$

As a consequence the viscous dissipation takes the form

$$\tilde{t}_{ij}A_{ij} - \tilde{g}_i^n N_i - \tilde{g}_i^m M_i \geqslant 0, \tag{2.10}$$

from which it readily follows that

$$\gamma_1 > 0, \quad \lambda_1 > 0, \quad \gamma_1 + \gamma_3 + \lambda_1 > 0. \tag{2.11}$$

Finally there are three Onsager relations

$$\gamma_2 = \alpha_3 + \alpha_2, \quad \lambda_2 = \beta_3 + \beta_2, \quad \gamma_4 = \mu_2 + \mu_1, \tag{2.12}$$

which reduce the number of independent viscous coefficients to twelve.

Continuum theory for uniaxial nematics follows from the above by setting all the β and μ coefficients in (2.5) equal to zero, and also corresponding terms in W, this eliminating the second director $\mathbf{m}$.

3. FLOW ALIGNMENT IN NEMATICS

The possible responses of a uniaxial nematic to shear flow are well known, but for completeness it is useful to give a brief summary here. To fix ideas consider a simple shear flow in which referred to Cartesian axes

$$v_x = kz, \quad v_y = v_z = 0, \tag{3.1}$$

where k is a positive constant. At most two steady configurations are possible, either

$$n_x = n_z = 0, \quad n_y = 1, \tag{3.2}$$

or provided that the coefficients α_2 and α_3 have the same sign

$$n_x = \cos\theta_o, \quad n_y = 0, \quad n_z = \pm\sin\theta_o, \tag{3.3}$$

the acute angle θ_o defined by

$$\tan^2\theta_o = \alpha_3/\alpha_2. \tag{3.4}$$

The solution (3.2) is always unstable, and on account of the condition (2.11) the solutions (3.3) lead to two cases, namely

$$\text{(i)}\ \alpha_2 < \alpha_3 < 0, \quad \text{and} \quad 0 < \theta_o < \pi/4,$$

$$\text{(ii)}\ \alpha_3 > \alpha_2 > 0, \quad \text{and} \quad \pi/4 < \theta_o < \pi/2. \tag{3.5}$$

For the former, the solution with n_z positive is stable, the other unstable, and for the latter the solution with n_z negative is stable, the other unstable. The former of course describes the behaviour of "rod-like" nematics, and while the latter has largely been ignored, Carlsson [6, 7] anticipates that it may well describe the response of discotic nematics, this prompted by some microscopic calculations by Forster [4] and Volovic [5].

In a recent paper Leslie [13] discusses flow alignment of biaxial nematics in some detail, and for the flow (3.1) finds three possible equilibrium configurations as follows:

$$S_m: m_x = m_z = 0, m_y = 1, \ n_x = \cos\theta, n_y = 0, \ n_z = \sin\theta,$$

$$\tau_1 \cos 2\theta + 1 = 0, \ \tau_1 = \gamma_2/\gamma_1; \tag{3.6}$$

$$S_n: n_x = n_z = 0, n_y = 1, \ m_x = \cos\phi, m_y = 0, m_z = \sin\phi,$$

$$\tau_2 \cos 2\phi + 1 = 0, \ \tau_2 = \lambda_2/\lambda_1; \tag{3.7}$$

$$S_\ell: n_x = \cos\psi, n_y = 0, n_z = \sin\psi, m_x = \sin\psi, m_y = 0, m_z = -\cos\psi,$$

$$\tau_3 \cos 2\psi + 1 = 0, \ \tau_3 = (\gamma_2 + \gamma_4 - \lambda_2)/(\gamma_1 + \gamma_3 + \lambda_1). \tag{3.8}$$

Moreover, he is able to show that in general these are the only equilibrium solutions available, and proceeds to show that at most only one of the above six solutions is stable, the particular solution dependent upon the particular values of the viscous coefficients. Of his results we are interested here simply in two limiting cases, one being that approaching a uniaxial microstructure and the other a discotic structure.

The uniaxial limit is obtained by allowing the β and μ coefficients to tend to zero, with the result that τ_3 tends to τ_1, with the behaviour of τ_2 unknown. Assuming that τ_1 and so τ_3 have magnitude greater than unity, stability considerations then eliminate the S_n option if the magnitude of τ_2 is greater than unity, and one obtains either S_m or S_ℓ governed by

$$S_m: \tau_1 > 1, \tau_3 > 1, \tau_2 > \tau_2^c, \quad \text{or} \quad \tau_1 < -1, \tau_3 < -1, \tau_2 < \tau_2^c;$$

$$S_\ell: \tau_1 > 1, \tau_3 > 1, \tau_2 < \tau_2^c, \quad \text{or} \quad \tau_1 < -1, \tau_3 < -1, \tau_2 > \tau_2^c; \tag{3.9}$$

where the value τ_2^c is given by

$$\tau_2^c = (\tau_3 - \tau_1)/(\tau_1 \tau_3 - 1). \tag{3.10}$$

The choice of the two available solutions in each configuration is dictated by

$$S_m: \quad \tau_1 \sin 2\theta < 0; \quad S_\ell: \quad \tau_3 \sin 2\psi < 0. \tag{3.11}$$

Hence in this limit, the outcome is essentially the same, whatever the values of τ_2, the **n** director is in the plane of shear at the same angle to the streamlines, with the secondary director either normal to the shear plane, or within this plane. Thus the alignment is basically that of a uniaxial nematic.

Of greater interest, however, is the second limit in which the β coefficients tend to their α counterparts, and γ_4 and γ_3 both tend to zero (this limit is discussed more fully in the following section). As a consequence τ_2 tends to τ_1 and τ_3 tends to zero in this limit. Again assuming that both τ_1 and τ_2 have magnitudes greater than unity, the configuration S_ℓ is not an option when the magnitude of τ_3 is less than unity and the choice between S_n or S_m is governed by

$$S_n: \tau_1 > 1, \tau_2 > 1, \tau_3 < \tau_3^c, \quad \text{or} \quad \tau_1 < -1, \tau_2 < -1, \tau_3 > \tau_3^c;$$

$$S_m: \tau_1 > 1, \tau_2 > 1, \tau_3 > \tau_3^c, \quad \text{or} \quad \tau_1 < -1, \tau_2 < -1, \tau_3 < \tau_3^c; \qquad (3.12)$$

where the value τ_3^c is defined by

$$\tau_3^c = (\tau_2 - \tau_1)/(\tau_1 \tau_2 - 1), \qquad (3.13)$$

and clearly is close to zero. The particular solution in each configuration is dictated by

$$S_m: \tau_1 \sin 2\theta < 0; \quad S_n: \tau_2 \sin 2\phi < 0. \qquad (3.14)$$

Thus, if τ_1 and τ_2 are both less than minus one, either **n** or **m** aligns as in a uniaxial "rod-like" nematic, with the second director perpendicular to the plane of shear, each one's role determined by the relative magnitudes of τ_1 and τ_2. These conclusions largely support Carlsson's [6, 7] conjecture regarding a uniaxial description of discotic nematics, but we return to this in the next section. Similarly, if both τ_1 and τ_2 are greater than unity, the behaviour of **n** or **m** is as predicted for a discotic nematic, with the other normal to the shear plane.

4. DISCOTIC NEMATICS

As discussed earlier a discotic nematic is one extreme or limit of a biaxial nematic, in which the major and minor axes of the elliptic platelet become indistinguishable. Here, therefore, we examine the theory for a biaxial nematic given in section 2, when the two directors **n** and **m** become physically indistinguishable. In this event, one naturally sets

$$\beta_1 = \alpha_1, \beta_2 = \alpha_2, \beta_3 = \alpha_3, \beta_5 = \alpha_5, \beta_6 = \alpha_6,$$

$$\mu_4 = \mu_3, \mu_2 = \mu_1 = 0, \tag{4.1}$$

the latter a consequence of the Onsager relations (2.12). With these assumptions, it seems reasonable to attempt to eliminate the directors **n** and **m** from the equation (2.5) in favour of a single director ℓ, the third member of the orthonormal triad.

Noting the well known identity

$$n_i n_j + m_i m_j + \ell_i \ell_j = \delta_{ij}, \tag{4.2}$$

one can clearly write

$$A_{ip} n_p n_j + A_{ip} m_p m_j + A_{ip} \ell_p \ell_j = A_{ij}, \tag{4.3}$$

allowing the elimination of the directors **n** and **m** from the terms with coefficients α_5 and α_6. Further introducing the local angular velocity **w** and a relative rate of rotation $\boldsymbol{\omega}$ by

$$\omega_i = \mathrm{w}_i - 1/2 e_{ijk} v_{k,j}, \tag{4.4}$$

the vectors **N** and **M** defined in (2.6) can be expressed as

$$N_i = e_{ipq} \omega_p n_q, \quad M_i = e_{ipq} \omega_p m_q. \tag{4.5}$$

Similarly, one can introduce a vector **L** associated with ℓ such that

$$L_i = e_{ipq} \omega_p \ell_q = \frac{d}{dt} \ell_i - W_{ip} \ell_p. \tag{4.6}$$

Hence, with the aid of (4.2), it quickly follows that

$$N_i n_j + M_i m_j + L_i \ell_j = e_{ipq} \omega_p \delta_{qj} = e_{ipj} \omega_p. \tag{4.7}$$

However, noting a further identity

$$\delta_{pq} e_{ijr} = \delta_{pi} e_{qjr} + \delta_{pj} e_{iqr} + \delta_{pr} e_{ijq}, \tag{4.8}$$

a contraction of this with $\ell_p \ell_q \omega_r$ leads to

$$e_{ijr}\omega_r = \ell_i e_{qjr}\ell_q\omega_r + \ell_j e_{iqr}\ell_q\omega_r + \ell_p\omega_p e_{ijq}\ell_q$$
$$= L_j\ell_i - L_i\ell_j + e_{ijq}\ell_q\ell_p\omega_p. \tag{4.9}$$

Hence, combining (4.7) and (4.9), one obtains

$$N_i n_j + M_i m_j = -L_j\ell_i - e_{ijq}\ell_q\ell_p\omega_p, \tag{4.10}$$

allowing the elimination of **n** and **m** from terms with coefficients α_2 and α_3.

Straightforwardly with the identity (4.2) and incompressibility one has

$$n_p n_q A_{pq} + m_p m_q A_{pq} + \ell_p\ell_q A_{pq} = 0, \tag{4.11}$$

and employing this twice it follows that

$$n_p n_q A_{pq} n_i n_j + m_p m_q A_{pq} m_i m_j$$
$$= \ell_p\ell_q A_{pq}(\ell_i\ell_j - \delta_{ij}) - m_p m_q A_{pq} n_i n_j - n_p n_q A_{pq} m_i m_j. \tag{4.12}$$

Also, as noted by Govers and Vertogen[10] use of (4.2) as indicated on

$$\ell_i\ell_j\ell_k\ell_p A_{kp} = (\ell_i\ell_j)(\ell_k\ell_p)A_{kp} = (\ell_i\ell_k)(\ell_j\ell_p)A_{kp} \tag{4.13}$$

leads to the relationship

$$n_p n_q A_{pq} m_i m_j + m_p m_q A_{pq} n_i n_j - n_p m_q A_{pq}(n_i m_j + n_j m_i)$$
$$= A_{ij} - A_{ip} n_p n_j - A_{jp} n_p n_i - A_{jp} m_p m_i - A_{ip} m_p m_j$$
$$+ (n_p n_q A_{pq} + m_p m_q A_{pq})\delta_{ij}. \tag{4.14}$$

By combining (4.12) and (4.14) and choosing

$$\mu_4 = \mu_3 = \alpha_1, \tag{4.15}$$

one can eliminate **n** and **m** from the terms with coefficient α_1.

Consequently, absorbing multiples of the Kronecker delta into the arbitrary pressure in (2.4), the viscous stress (2.5) reduces to

$$\tilde{t}_{ij} = \eta_1 \ell_p \ell_q A_{pq} \ell_i \ell_j + \eta_2 L_i \ell_j + \eta_3 L_j \ell_i + \eta_4 A_{ij}$$

$$+ \eta_5 A_{ip} \ell_p \ell_j + \eta_6 A_{jp} \ell_p \ell_i + \eta_7 e_{ijp} \ell_p \ell_k \omega_k, \tag{4.16}$$

where

$$\eta_1 = \alpha_1, \eta_2 = -\alpha_3, \eta_3 = -\alpha_2, \eta_4 = \alpha_4 + \alpha_5 + \alpha_6 + \alpha_1,$$

$$\eta_5 = -\alpha_5 - \alpha_1, \eta_6 = -\alpha_6 - \alpha_1, \eta_7 = \alpha_3 - \alpha_2. \tag{4.17}$$

The final term in (4.16) may prove to be of no consequence on account of the equation of angular momentum as Leslie [14] discusses, but alternatively one might simply choose to ignore such a contribution given that the component of spin normal to the disc is hardly likely to be detectable.

While the above outcome is not altogether surprising, it is reassuring to note the consistency between the different approaches. A discotic nematic regarded as a limit of a biaxial platelet that aligns at a small angle to the streamlines, leads to the appropriate uniaxial model anticipated by Carlsson[6, 7], namely a uniaxial nematic with its α_2 and α_3 coefficients both positive.

References

[1] J. L. Ericksen, *Trans. Soc. Rheol.*, **5**, 23 (1961).
[2] F. M. Leslie, *Arch. Ration. Mech. Anal.*, **28**, 265 (1968).
[3] F. M. Leslie, *Mol. Cryst. Liq. Cryst.*, **63**, 111 (1981).
[4] D. Forster, *Phys. Rev. Lett.*, **32**, 1161 (1974).
[5] G.E. Volovic, *JETP Lett.*, **31**, 273 (1980).
[6] T. Carlsson, *Mol. Cryst. Liq. Cryst.*, **89**, 57 (1982).
[7] T. Carlsson, *J. Physique*, **44**, 909 (1983).
[8] L. J. Yu and A. Saupe, *Phys. Rev. Lett.*, **45**, 1000 (1980).
[9] A. Saupe, *J. Chem. Phys.*, **75**, 5118 (1981).
[10] E. Govers and G. Vertogen, *Physica A*, **133**, 337 (1985).
[11] A. Chauré, *Int. J. Engng. Sci.*, **23**, 797 (1985).
[12] F. M. Leslie, J. S. Laverty and T. Carlsson, *Q. Jl. Mech. Appl. Math.*, **45**, 595 (1992).
[13] F. M. Leslie, *J. Non-Newton. Fl. Mech.*, **54**, 241 (1994).
[14] F. M. Leslie, *Continuum Mech. Thermodyn.*, **4**, 167 (1992).