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On the flow-phase diagram for discotic liquid crystals in uniaxial extension and compression

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A mesoscopic, extended Doi theory for flows of nematic liquid crystals (LCs) has been successfully applied by Rey to study extensional flow-induced, homogeneous phase transitions both for rod-like and disc-like molecular geometry. Rey analysed the two order parameters (eigenvalues) of the orientation tensor. Recently the authors generalized the flow-phase diagram (nematic concentration vs. flow rate) for rod-like nematics by analysing all tensor degrees of freedom, i.e. by coupling the three director (eigenvector) degrees of freedom. Here we record and discuss subtleties of the corresponding diagram for discotic LCs in uniaxial extension and uniaxial compression. We focus here on the induced stable orientation configurations. Uniaxial extension (an idealization of fibre flow) yields a low concentration region of unique oblate uniaxial states at every flow rate; a very small finite region of bi-stable oblate and biaxial states; and the predominant region, encompassing all concentrations above the pure I–N transition and all flow rates, where the only stable steady state is a biaxial pattern. Furthermore, whereas uniaxial states are 'unique', all biaxial states occur in a continuous family, corresponding to an arbitrary positioning of the director pair in the plane transverse to the flow axis of symmetry. Uniaxial compression (an idealization of film stretching flow) of discotic LCs exclusively yields stable prolate uniaxial patterns.

From Rey [1], the mesoscale orientation of discotic nematic LCs may be described by a rank 2, symmetric, traceless tensor **Q**. We assume simple extensional flow defined by a velocity field.

$$\mathbf{v} = v\left(-\frac{x}{2}, -\frac{y}{2}, z\right) \tag{1}$$

where

$$\nabla\mathbf{v} = v \text{ diag}\left(-\frac{1}{2}, -\frac{1}{2}, 1\right). \tag{2}$$

For $v > 0$, the flow stretches along the z-axis (uniaxial extension); for $v < 0$, the flow stretches radially in the entire plane orthogonal to the z-axis (uniaxial compression).

The extended Doi theory [2] admits a molecular shape parameter, β, given by

$$\beta = \frac{p^2 - 1}{p^2 + 1} \tag{3}$$

where p is the aspect ratio of an idealized molecular oblate spheroid; $p = 1, 0, \infty$ correspond to a sphere, flat disc, and cylindrical rod, respectively. For discotic LCs, we fix $0 < p < 1$, or $-1 < \beta < 0$.

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With the velocity field (1) rigidly enforced, the extended Doi theory for flows of discotic LCs reduces to a flow perturbed tensor ode for $\mathbf{Q}$ in dimensionless form [1]:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} = -\mathbf{F}(\mathbf{Q}) + \beta v \lambda \mathbf{G}(\mathbf{Q}; \tilde{\mathbf{D}}) \\ \mathbf{F}(\mathbf{Q}) = (1 - N/3)\mathbf{Q} - N(\mathbf{Q}\;\mathbf{Q}) + N(\mathbf{Q} : \mathbf{Q})(\mathbf{Q} + \mathbf{I}/3) \\ \mathbf{G}(\mathbf{Q}; \tilde{\mathbf{D}}) = \tilde{\mathbf{D}}\mathbf{Q} + \mathbf{Q}\tilde{\mathbf{D}} + \dfrac{2}{3}\tilde{\mathbf{D}} - 2\tilde{\mathbf{D}} : \mathbf{Q}\left(\mathbf{Q} + \dfrac{\mathbf{I}}{3}\right) \end{cases} \tag{4}$$

where the dimensionless velocity gradient $\tilde{\mathbf{D}}$, from (2), is constant,

$$\tilde{\mathbf{D}} = \mathrm{diag}(-1/2, -1/2, 1), \quad \hat{t} = t/\lambda \tag{5}$$

λ is the elastic relaxation time of the LC, and N is a dimensionless concentration parameter. The term $\mathbf{F}(\mathbf{Q})$ corresponds to a short-range, Maier–Saupe, excluded-volume interaction, while $\mathbf{G}$ captures the flow-induced nematic response. Since we restrict this treatment to homogeneous phase transitions in simple steady flow, the long-range distortional potential is neglected as in [3–5].

For rod-like (prolate spheroid) nematics, $0 < \beta \leq 1$, the results from [3] apply directly with only a scaling of $v\lambda$ by β. For discotic nematic LCs, $-1 < \beta < 0$, the flow-phase diagram for flow rate (v) vs concentration (N) is achieved by mirror reflection about $v = 0$ of the diagram in [3]. The analysis in [3] relies heavily on the following tensor basis:

$$\mathbf{Q}^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}, \quad \mathbf{Q}^{(2)} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{Q}^{(3)} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{6}$$

$$\mathbf{Q}^{(4)} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{Q}^{(5)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{7}$$

which provides tensorial eigenfunctions for linearization about all equilibria. From [3, 5] these basis elements correspond to the following homogeneous modes, $\mathbf{Q}^{(1)}$ is a *splay* mode with respect to the flow axis of symmetry $\mathbf{e}_z$, $\mathbf{Q}^{(2)}$ and $\mathbf{Q}^{(3)}$ are *twist* modes, $\mathbf{Q}^{(4)}$ and $\mathbf{Q}^{(5)}$ are *bend* modes. $\mathbf{Q}^{(1)}$, $\mathbf{Q}^{(2)}$ are equivalent to the order parameter degrees of freedom; $\mathbf{Q}^{(3)}$, $\mathbf{Q}^{(4)}$, $\mathbf{Q}^{(5)}$ capture the 'director' or optical axes degrees of freedom.

Making this correspondence with [3], we deduce the extensional flow-phase diagram for discotic LCs, figure 1, where $-1 < \beta < 0$. In figure 1, the Peclet number $Pe = |\beta| v\lambda > 0$ corresponds to uniaxial *extension* and $Pe < 0$ corresponds to uniaxial *compression*. Note that the curve CI that separates regimes VI, VII is not given in [1]. There are many coexisting uniaxial and biaxial steady states in each region; here we report only those that are stable or neutrally stable in tables 1 and 2. Additional unstable states, and their tensor modes of instability, are given in [3].

The characterization of discotic mesophase orientation is given in terms of the eigenvalues d_i (order parameters) and eigenvectors $\mathbf{n}_i$ (directors) of $\mathbf{Q}$. It is important to remember that the molecular direction $\mathbf{m}$ of a disc-like molecule is the normal to the disc. The eigenvalues of $\mathbf{Q}$, $d_i = \cos^2(\angle(\mathbf{n}_i, \mathbf{m}))$, $0 \leq d_i \leq 1$, $\Sigma_{i=1}^{3} d_i = 1$, provide

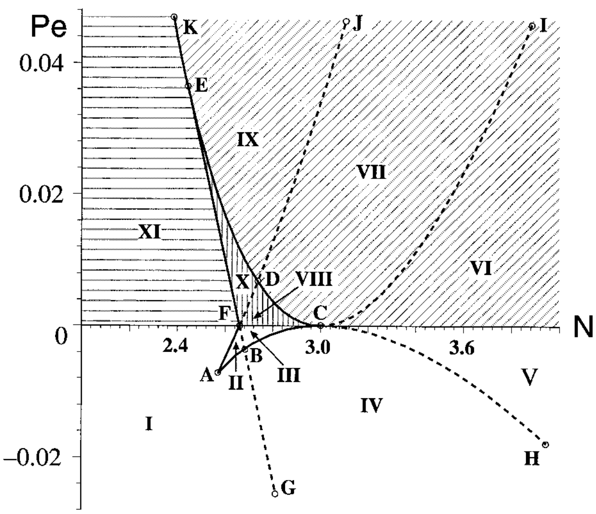

Figure 1. Flow-phase diagram for extensional flow of discotic LCs with molecular shape parameter $-1 \leq \beta < 0$, and fixed relaxation time λ. The vertical axis is the effective Peclet number, $Pe = |\beta| v\lambda$. $Pe > 0$ corresponds to uniaxial extension, $Pe < 0$ to uniaxial compression.

Table 1. A catalogue of co-existing stable or neutrally stable steady states of discotic LCs in *uniaxial extension.*

Region	Type of states
VI	B
VII	B
VIII	B, O
IX	B
X	B, O
XI	O

Table 2. A catalogue of co-existing stable steady states of discotic LCs in *uniaxial compression*.

Region	Type of states
I	P
II	P^1, P^2
III	P^1, P^2
IV	P
V	P

the birefringence with respect to the optical axes $\mathbf{n}_i$, equivalently directors, equivalently eigenvectors, of $\mathbf{Q}$. The spectral decomposition of $\mathbf{Q}$ is

$$\mathbf{Q} = \sum_{i=1}^{3} \left(d_i - \frac{1}{3} \right) \mathbf{n}_i \otimes \mathbf{n}_i. \quad (8)$$

The birefringence in the plane of $\mathbf{n}_i$, $\mathbf{n}_j$ is $|d_i - d_j|$. Isotropic structure corresponds to $d_1 = d_2 = d_3 = 1/3$; uniaxiality corresponds to one simple eigenvalue d_i, with $d_j = d_k$, $i \neq j \neq k$ and isotropy in the plane orthogonal to $\mathbf{n}_i$; prolate uniaxiality corresponds to $d_i > 1/3$, so that the molecule normals, $\mathbf{m}$, on average are tilted toward the distinguished optical axis $\mathbf{n}_i$; oblate uniaxiality corresponds to $0 \leqslant d_i < 1/3$. Biaxiality corresponds to $d_i \neq 1/3$, $d_i \neq d_j$, for any i, j.

The new information provided here relates to Regions VI, VII where a prolate uniaxial state in each region suffers two director instabilities (eigenvectors $\mathbf{Q}^{(4)}$, $\mathbf{Q}^{(5)}$) not resolved in [1]. Thus no stable uniaxial states exist in these parameter regimes or Region IX. These unstable modes are the extensional flow analogues of shear-induced tumbling modes.

The main results for discotic LC mesophases can be summarized as follows.

In *uniaxial extension* ($Pe > 0$):

(1) The only stable uniaxial discotic phases are oblate, denoted by O in table 1, in the low-to-moderate concentration regions to the left of the phase transiton curve KEDC. This means that the plane of discotic molecules on average tilts toward the flow extension axis; the degree of tilt (d_3) is proportional to Pe, i.e. the flow rate.

(2) A neutrally stable biaxial state (denoted B in table 1) is the unique orientation structure everywhere to the right of the phase transition curve KEDC, with $Pe > 0$. The degrees of orientation, i.e. the order parameters, vary continuously as functions of N and Pe. Each pattern B corresponds to a continuous family of patterns, with the directors in the x–y plane not selected from the physics of this model. This translates to one zero linearized eigenvalue of each fixed biaxial state, with linearized tensorial eigenfunction, $\mathbf{Q}^{(3)}$.

(3) The small region between curves KEDC and EF has bi-stable states, one oblate (O) and one biaxial (B). This is the *only* parameter region of bi-stability, which is the remnant of the pure nematic bi-stable concentrations $8/3 < N < 3$, segment FC along $Pe = 0$ in figure 1.

(4) The low concentration region XI has only a unique stable oblate uniaxial phase (O), for all flow rates $v > 0$ and concentrations left of KEF in figure 1.

(5) Crossing EF from left to right, a neutrally stable biaxial state appears and the oblate state remains stable. Crossing FK from left to right, the stable oblate state becomes unstable and a neutrally stable biaxial state appears. Crossing CDE from left to right, the stable oblate state becomes unstable and the neutrally stable biaxial state remains. Crossing FDJ or CI from left to right, the stable states are unchanged while all states participating in the transition are unstable. In other words, FDJ and CI are mathematical bifurcations which are restricted to unstable equilibria. From an experimental point of view, the bifurcation curves are FEK and CDEK.

In figure 2 we depict the geometrical representation of the mesoscopic orientation tensor for fixed flow rate $Pe = 0.04$ while varying the concentration (equivalently, temperature).

In *axial compression* ($Pe < 0$), relevant for film stretching-type flows of discotic LCs, the only stable patterns are uniaxial prolate phases, denoted by P or P^i in table 2. All uniaxial states are discrete, with the distinguished director aligned with the flow axis of symmetry. Again, in figure 1 the experimental boundaries are AF and ABC, whereas FBG and CH are 'ghost' phase transition curves restricted to unstable equilibria which have no bearing in the experimental bifurcation.

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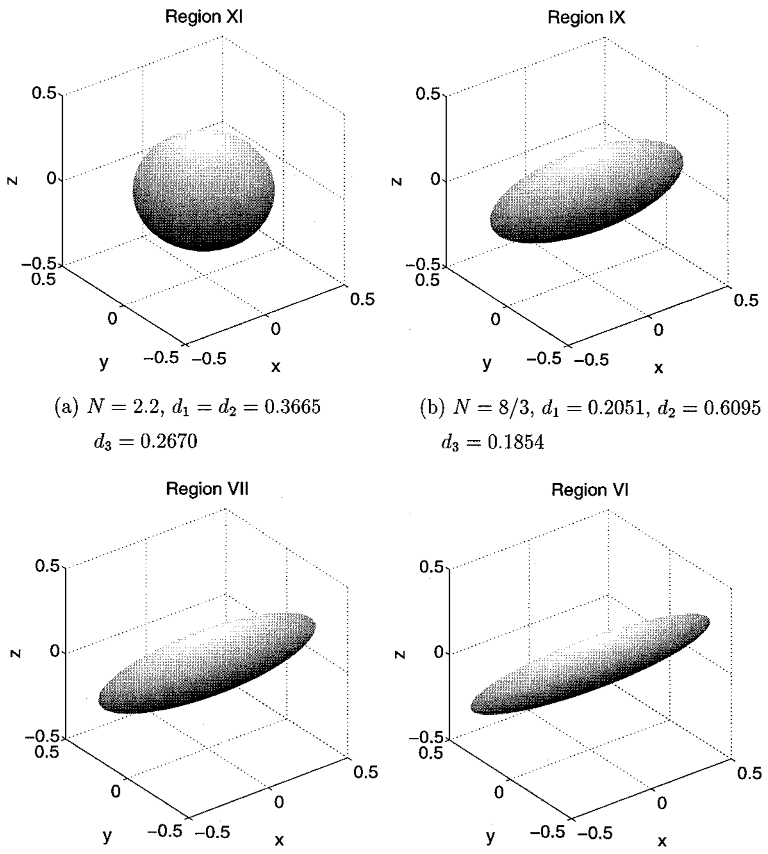

(a) $N = 2.2$, $d_1 = d_2 = 0.3665$ $d_3 = 0.2670$

(b) $N = 8/3$, $d_1 = 0.2051$, $d_2 = 0.6095$ $d_3 = 0.1854$

(c) $N = 3.3$, $d_1 = 0.1380$, $d_2 = 0.7318$ $d_3 = 0.1302$

(d) $N = 3.9$, $d_1 = 0.1085$, $d_2 = 0.7876$ $d_3 = 0.1038$

Figure 2. Geometrical representation of the mesoscopic orientation tensor in uniaxial extension where $Pe = 0.04$ is fixed and the concentration N varies. The order parameters determine the degrees of orientation, d_i, which are the semi-axis lengths. One director is always fixed $\mathbf{n}_3 = \mathbf{e}_z$ parallel to the flow; the remaining directors $\mathbf{n}_1$, $\mathbf{n}_2$ are arbitrary, given here as unit coordinate vectors.

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