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Analysis of Thermal Instabilities in Uniformly Aligned Cholesteric Liquid Crystals

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This paper employs continuum theory to examine the onset of a particular type of cellular thermal convection when a long pitch cholesteric liquid crystal between two infinite horizontal flat plates is subject to a vertical temperature gradient. The initial alignment considered is uniform and either perpendicular or parallel to the plane of the plates. A Fourier series method is used to investigate the influence of the pitch of the cholesteric on the critical threshold gradient at which each of the initial alignments becomes unstable.

1. INTRODUCTION

There has been a substantial growth in the study of thermally induced flow phenomena in liquid crystals during the last ten years. The first theoretical investigations by Dubois-Voilette[1] and Currie[2] consisted of relatively simple analyses of the Bénard convection problem for a nematic liquid crystal. The qualitative predictions for their approximate calculations were soon confirmed by experiment, including the novel result that convective motion can occur in particular cases when the sample is heated from above. These initial studies have stimulated several more detailed theoretical and experimental investigations of roll-type stationary instabilities in nematic liquid crystals which are comprehensively reviewed by Leslie.[3] Details of the related analyses of oscillatory instabilities in nematics are available in the paper by Guyon *et al.*[4]

By way of contrast, there have been significantly fewer investigations of thermal flow phenomena in cholesteric liquid crystals. One reason for this is that the continuum theory for this class of liquid crystal is more complex, partly due to the inherent twisted structure of these materials, but also because the weaker symmetries in cholesterics allow more coupling in the equations. The calculation by Dubois-Voilette[5] appears to be the only attempt to analyze Bénard convection in cholesteric liquid crystals. Her analysis makes several simplifying assumptions; in particular, she considers materials with small pitch and also neglects the thermomechanical coupling terms discussed by Leslie[6,7] on the grounds that they may play a secondary rôle in this phenomenon. However, in this case, the availability of a theoretical analysis does not appear to have stimulated an associated experimental investigation. This is somewhat surprising, and equally strange is the absence of experimental studies of the thermomechanical coupling effects discussed by Leslie.

Given that the inherent twisted configuration of a cholesteric tends to lead to complex theoretical calculations, the present paper considers situations in which this complication is absent, and discusses cases involving uniformly aligned cholesterics. These may occur naturally between parallel plates if the cholesteric liquid crystal has a sufficiently long pitch or the gap width is sufficiently small,[8] and therefore we discuss the opposite limit from Dubois-Voilette.[5] Consequently, we examine the stability of planar and homeotropically aligned cholesterics between horizontal plates in the presence of a vertical temperature gradient. Our analysis employs a Fourier series method due to Jeffreys[9] to obtain an exact expression for the threshold gradient for a cholesteric liquid crystal in the situations described above.

In this preliminary investigation, we follow Dubois-Voilette[5] and choose to ignore the additional thermomechanical coupling terms in the cholesteric equations. The absence of experimental data regarding these coupling terms prompts us to assume that they may be of secondary importance in this context. On the other hand, conflict between the predictions of this analysis and experiment would prove this assumption to be ill-founded. In any event, one hopes that the existence of further theoretical predictions will promote associated experimental investigations of these flow phenomena in cholesterics.

2. FORMULATION OF THE PROBLEM

In this paper we assume that the equations governing the behavior of an incompressible cholesteric liquid crystal are those proposed by Leslie,[3] and use them to examine the stability of a cholesteric sample confined between two horizontal infinite flat plates in the presence of a vertical temperature gradient. With an appropriate choice of Cartesian axes, the upper plate is situated at $z = h$ and the lower at $z = 0$, their temperatures being maintained at the constant values T_U and T_L respectively. Our analysis considers two particular situations in which the initial alignment is uniform, either planar or homeotropic due to appropriate prior treatment of the plates.

Assuming that the external body force arises only from gravity, we adopt the forms for the body force and couple proposed by Ericksen,[10] and look initially for static equilibrium solutions in which the unit vector $\mathbf{n}$ describing the alignment of the anisotropic axis takes its boundary value throughout the sample. In this event, the governing equations yield the following expressions for the temperature T and the pressure p,

$$T = T_L + \phi z, \qquad \phi = (T_U - T_L)/h, \qquad p = p_0 - g\int \rho\, dz, \tag{2.1}$$

where p_0 is an arbitrary constant, g is the acceleration due to gravity and ρ is the density. From comparison with the energies of twisted states,[8] these uniform alignments of cholesterics certainly require samples with sufficiently long pitch P, or rather small gap width h, satisfying

$$P \geqslant 4h, \tag{2.2}$$

and thus the subsequent analysis assumes that these parameters satisfy the above necessary condition.

If the equilibrium state is slightly disturbed, we consider a small amplitude velocity $\mathbf{v}$, an associated perturbed director $\mathbf{n} + \mathbf{d}$, a temperature $T + s$, a pressure $p + \bar{p}$ and a director tension $\bar{\gamma}$. In the subsequent linearization of the governing equations about the equilibrium state, it seems reasonable to adopt the usual Boussinesq approximation,[11] which ignores all variations of the material parameters except where associated with gravity. As a consequence the linearized equations take the form

$$v_{i,i} = 0, \qquad n_i d_i = 0, \tag{2.3}$$

$$\rho\frac{\partial v_i}{\partial t} = -\rho' g s k_i - \bar{p}_{,i} - K_2\tau e_{jkl} n_l d_{k,ij} + A_{ijkm} v_{j,km} + B_{ijk}\frac{\partial d_{j,k}}{\partial t} \qquad \rho' = \frac{\partial \rho}{\partial T}, \tag{2.4}$$

$$\sigma\frac{\partial^2 d_i}{\partial t^2} = \bar{\gamma} n_i - 2K_2\tau e_{ijk} d_{k,j} + C_{ijkm} d_{j,km} + D_{ijk} v_{j,k} - \gamma_1\frac{\partial d_i}{\partial t}, \tag{2.5}$$

$$C\left(\frac{\partial s}{\partial t} + \phi v_i k_i\right) = -\kappa_1 s_{,ii} - \kappa_2 n_i n_j s_{,ij} - \phi\kappa_2 k_j (n_i d_{j,i} + n_j d_{i,i}), \tag{2.6}$$

where K_2, τ, σ, γ_1, κ_1, κ_2 are material parameters,[3] C the specific heat at constant volume, and $\mathbf{k}$ the unit vector in the z-direction. The coefficients

A_{ijkm}, B_{ijk}, C_{ijkm} and D_{ijk} are essentially those given by Currie[2] and are listed in Appendix I. It is convenient to note at this point that the pitch P and the material parameter τ are related by

$$P = \frac{2\pi}{|\tau|}. \tag{2.7}$$

3. INITIAL HOMEOTROPIC ALIGNMENT

In the case of homeotropic alignment, the unit vector $\mathbf{n}$ is in the z-direction and the symmetry of the problem permits an arbitrary choice of orientation for the x-axis. We consider perturbations in the form of rolls, and with an appropriate choice of x-axis, therefore examine without loss of generality disturbances of the form

$$\mathbf{d} = (d_1, d_2, 0)\exp(imx + \nu t), \qquad \mathbf{v} = (u, v, w)\exp(imx + \nu t),$$
$$\bar{p} = \bar{p}\exp(imx + \nu t), \qquad s = s\exp(imx + \nu t), \tag{3.1}$$

where $d_1, d_2, u, v, w, \bar{p}$ and s are functions of z alone. Appropriate boundary conditions to be applied at $z = 0$ and $z = h$ are

$$d_1 = d_2 = u = v = w = s = 0. \tag{3.2}$$

Our aim is to find the smallest absolute value of the temperature difference ϕh at which these disturbances become unstable for all possible values of the wavenumber m. In line with similar studies, we adopt the principle of exchange of stabilities[12] and assume that for each value of m the onset of instability is characterized by ν being identically zero. With this assumption, substitution of Eqs. (3.1) into Eqs. (2.3)–(2.6) yields a system of linear differential equations, one of which with the boundary condition $(3.2)_4$ implies that the y-component of the perturbed velocity field vanishes identically; thus one finds that the convective instability is confined to the (x, z) plane. However, non-zero values for τ permit the perturbed director field $\mathbf{d}$ to have a component in the y-direction, and in this respect the present analysis differs from the corresponding nematic problem[13,14] in which the perturbation velocity and director fields are both confined to one plane.

Elimination of d_1, d_2, u, $\bar{p}$ and s from the system of equations, and the change of variable

$$\xi = \pi z/h, \tag{3.3}$$

yields a tenth order equation for w,

$$(D^2 - \kappa a^2)(D^4 - \eta a^2 D^2 + \eta_1 a^4)[(D^2 - l_1 a^2)(D^2 - l_2 a^2) + l_3 D^2]w$$
$$= -R[(D^2 - l_2 a^2)(D^2 + \lambda a^2) + 2l_4 D^2]a^2 w, \qquad (3.4)$$

where $D \equiv d/d\xi$, $a = m\pi/h$ is a dimensionless wave number, and κ, η, η_1, l_1, l_2, l_3, l_4, λ and R are defined in Appendix II. The boundary conditions to be applied at both $\xi = 0$ and $\xi = \pi$ follow from Eqs. (3.2) and Eqs. (2.3)–(2.6), and take the form

$$w = Dw = D^2(D^2 - \eta a^2)w = D^2(D^4 - \eta a^2 D^2 + \eta_1 a^4)w$$
$$= D(D^2 - \kappa a^2)(D^2 - l_1 a^2 + l_3)$$
$$(D^4 - \eta a^2 D^2 + \eta_1 a^4)w + Ra^2 D^3 w = 0. \qquad (3.5)$$

It is possible to solve the above boundary value problem by a Fourier series method which is described in the following section.

Before turning to the solution of the above, it is of interest to note that τ appears in the differential equation and its boundary conditions in even powers, and therefore our results are insensitive to the sign of τ. Also, some insight into likely predictions can be obtained by a repetition of the two-dimensional normal mode analysis given by Pieranski *et al.*[15] The result of such an approximate investigation follows readily from Eq. (3.4) simply by choosing the unknown w to have the form

$$w = w_0 e^{ilz} = w_0 e^{iq\xi}, \qquad q = \frac{lh}{\pi}, \qquad (3.6)$$

where w_0 is a constant. After some manipulation, one obtains

$$R = \frac{(q^2 + \kappa a^2)(q^4 + \eta a^2 q^2 + \eta_1 a^4)[(q^2 + l_1 a^2)(q^2 + l_2 a^2) - l_3 q^2]}{a^2[(q^2 + l_2 a^2)(q^2 - \lambda a^2) - 2l_4 q^2]}, \qquad (3.7)$$

which differs from the corresponding expression for the nematic problem only by the inclusion of the terms l_3 and l_4. These additional terms unique to the cholesteric formulation are positive functions of $h^2\tau^2$, and for the values of the various parameters discussed in the last section

$$l_3 \gg l_4 > 0, \qquad 1 \gg \lambda > 0. \qquad (3.8)$$

From this, one readily sees that when q and a are of the same order of magnitude, the presence of τ reduces the likely magnitude of the Rayleigh number and thus the critical threshold for the instability. This essentially is a consequence of the fact that the terms introduced by the chirality play a destabilizing rôle in the director torque equations for such an analysis. Moreover, to first order in τh, the critical value varies as the square of this quantity.

4. SOLUTION OF THE PROBLEM BY JEFFRIES METHOD

This section presents an adaptation of the Fourier series approach developed by Jeffries[9] to solve the boundary value problem obtained in the previous section. Barratt and Bramley[16] have employed a rather similar version of this method in a Bénard problem for nematic liquid crystals. Detailed values of the various coefficients in the equations which follow are available in Appendix III.

With the initial assumption that

$$D^{10}w = \sum_{r=1}^{\infty} A_r \sin r\xi \tag{4.1}$$

repeated integration yields

$$w = \sum_{r=1}^{10} \frac{B_r(\frac{\pi}{2} - \xi)^{r-1}}{(r-1)!} + \sum_{r=1}^{\infty} \frac{A_r \sin r\xi}{r^{10}} \equiv P(\xi) + \sum_{r=1}^{\infty} \frac{A_r \sin r\xi}{r^{10}}, \tag{4.2}$$

where the B_r are constants of integration. Substitution of Eq. (4.2) into Eq. (3.4) gives

$$\sum_{r=1}^{\infty} \mu_r \sin r\xi = (D^{10} - Q_1D^8 + Q_2D^6 - Q_3D^4 + Q_4D^2 - Q_5)P(\xi) \equiv L(\xi), \tag{4.3}$$

where

$$\mu_r = Q(r)A_r/r^{10}, \tag{4.4}$$

$$Q(r) = r^{10} + Q_1r^8 + Q_2r^6 + Q_3r^4 + Q_4r^2 + Q_5, \tag{4.5}$$

the Q_i being defined in Appendix III, and it follows from Eq. (4.3) that

$$\mu_r = \frac{2}{\pi}\int_0^{\pi} L(\xi) \sin r\xi d\xi. \tag{4.6}$$

With the aid of Eq. (4.4), (4.5) and the identity

$$\begin{aligned} I_m &= \int_0^{\frac{\pi}{2}} \left(\frac{\pi}{2} - \xi\right)^m \sin r\xi d\xi \\ &= \frac{2}{r}\sum_{k=0}^{p} \frac{(-1)^k m!}{(m-2k)!}\left(\frac{\pi}{2}\right)^{m-2k}\left(\frac{1}{r}\right)^{2k}, \qquad m + r \text{ odd}, \\ &= 0, \qquad m + r \text{ even}, \end{aligned} \tag{4.7}$$

where p is the largest integer $\leqslant m/2$, a tedious calculation eventually yields

$$\mu_{2r} = \frac{1}{2r}\sum_{i=1}^{5} P_{2i}B_{2i}, \qquad \mu_{2r+1} = \frac{1}{(2r+1)}\sum_{i=1}^{5} P_{2i-1}B_{2i-1}, \tag{4.8}$$

with

$$P_{n+1} = \frac{4}{\pi}\sum_{k=0}^{q} \frac{(-1)^{k+1}}{(n-2k)!} Q_{5-k} J_{n-2k}, \quad n = 0, 1, 2, \ldots, 9, \tag{4.9}$$

where q is the largest integer $\leqslant n/2$. Expressions (4.8) together with Eqs. (4.4) and (4.5) essentially determine the coefficients A_r as linear combinations of the B_i. From Eqs. (4.8) and the boundary conditions (3.5), it is found that there are two types of solution, one even, in $(\pi/2 - \xi)$, and the other odd, the former containing coefficients B_{2i-1} and the latter B_{2i}. In other similar problems, it is common to find that the least stable mode is the symmetric solution, and so we confine our attention to this symmetric mode. This choice is confirmed below for the selected values of the various material parameters by an orthonormalization calculation (see Sec. 5).

For a symmetric solution, Eqs. (4.2) and $(4.8)_1$ imply that all the B_{2i} and, hence, all the μ_{2i} and A_{2i} are identically zero. Employing Eqs. $(4.8)_2$ and (4.4) in Eq. (4.2), and substitution of the resulting expression for w into the boundary conditions (3.5) gives a system of simultaneous equations for the B_{2i-1} of the form

$$\sum_{j=1}^{5} \Phi_{ij}B_{2j-1} = \sum_{j=1}^{5} \Psi_{ij}S_j, \quad i = 1, 2, \ldots, 5, \tag{4.10}$$

where Φ and Ψ are the (5×5) matrices defined in Appendix III and

$$S_i = \sum_{r=0}^{\infty} \frac{A_{2r+1}}{(2r+1)^{2i-1}}, \qquad i = 1, 2, \ldots, 5. \tag{4.11}$$

Solving the system (4.10) for B_{2i-1} and substitution for the μ_{2r+1} with the aid of Eq. (4.4) in Eq. $(4.8)_2$ gives

$$\frac{A_{2r+1}}{(2r+1)^9} = \sum_{j=1}^{5} \frac{P_{2j-1}}{Q(2r+1)} \cdot \sum_{k=1}^{5} K_{jk}S_k, \tag{4.12}$$

where

$$K_{jk} = \sum_{l=1}^{5} \Phi_{jl}^{-1}\Psi_{lk}. \tag{4.13}$$

Multiplication of both sides of Eq. (4.12) by $(2r + 1)^{10-2i}$, $i = 1, 2, \ldots,$ 5, and performing a summation over r yields

$$S_i = \sum_{j=1}^{5} G_{ij} \sum_{k=1}^{5} K_{jk} S_k, \qquad i = 1, 2, \ldots, 5, \tag{4.14}$$

where

$$G_{ij} = \sum_{r=0}^{\infty} \frac{P_{2j-1}(2r + 1)^{10-2i}}{Q(2r + 1)}. \tag{4.15}$$

Finally, for the system (4.14) to have a non-trivial solution for the S_i, we have the consistency condition

$$\det\left(\sum_{j=1}^{5} G_{ij} K_{jk} - \delta_{ik}\right) = 0. \tag{4.16}$$

For a specific cholesteric material and prescribed sample thickness, Eq. (4.16) is an equation relating ϕ and a. For a specific P/h and a, we now proceed to determine the value of $|\phi|$ with smallest magnitude for which condition (4.16) holds. Fixing P/h, we repeat the process for various values of a to obtain a neutral stability curve in the (a, ϕ) plane. The value of ϕ with smallest magnitude gives the dimensionless temperature gradient for the onset of the convective instabilities considered in this paper.

Details of our numerical results are given and discussed in the final section.

5. INITIAL PLANAR ALIGNMENT

When the initial uniform alignment is parallel to the plates, the earlier symmetry considerations no longer apply and one should now choose roll-type perturbations with a direction of roll-axis arbitrary in the (x, y) plane. However, in this general case, one cannot employ the Fourier series method of solution because it does not appear to be possible to derive appropriate boundary conditions in only one dependent variable. In order to make some progress towards a solution, we first consider two simpler situations where the roll axis is either parallel or perpendicular to the initial alignment.

Roll axis parallel to *n*

When perturbations are in the form of rolls parallel to the initial alignment, the equations reduce to those of the classical Bénard problem for a Newtonian fluid confined between two rigid boundaries[12] with a Rayleigh number including only the thermal conductivity $\kappa_\parallel$ and viscosity α_4. Consequently, for this particular case, the relevant results are readily obtainable from the Newtonian calculation,[12] and yield threshold values comparable with those for Newtonian fluids. This is in contrast to the much lower thresholds usually found for liquid crystals.[3]

Roll axis perpendicular to *n*

In this case the analysis essentially follows that for the corresponding nematic problem[13,14] and considers disturbances of the form

$$d = (0, d_2, d_3)\exp(imx + \nu t), \qquad v = (u, 0, w)\exp(imx + \nu t),$$
$$\bar{p} = \bar{p}\exp(imx + \nu t), \qquad s = s\exp(imx + \nu t), \tag{5.1}$$

where d_2, d_3, u, w, $\bar{p}$, and s are again functions of z alone. The boundary conditions are similar to Eqs. (3.2), and with the change of variable (3.3). The appropriate differential equation for w is readily derived from Eqs. (2.3)–(2.6) as

$$(D^2 - \kappa' a^2)(D^4 - \eta' a^2 D^2 + \eta_1' a^4)[(D^2 - l_1' a^2)(D^2 - l_2' a^2) + l_3' a^2]w$$
$$= -R'[(D^2 - l_2' a^2)(D^2 + \lambda' a^2) + 2l_4' a^2]a^2 w, \tag{5.2}$$

with boundary conditions

$$w = Dw = D^2(D^2 - \eta' a^2)w = D^2(D^4 - \eta' a^2 D^2 + \eta_1' a^4)w$$
$$= D^4(D^4 - \eta' a^2 D^2 + \eta_1' a^4)w + R' a^2 D^2 w = 0, \tag{5.3}$$

to be applied at $\xi = 0$ and $\xi = \pi$, where $a = m\pi/h$ and the dashed constants are defined in Appendix II. The presence of τ again allows the perturbed director to twist out of the plane of the rolls, although when τ vanishes one essentially recovers the corresponding nematic problem.[13,14]

In this case it is again possible to apply the method of the previous section to obtain the critical threshold instability. The values for the various coefficients in this calculation are also given in Appendix III.

Here also the parameter τ appears only in even powers and thus our results are again insensitive to the sign of τ. As earlier, a two-dimensional normal mode analysis leads to the following approximate result

$$R' = \frac{(q^2 + \kappa' a^2)(q^4 + \eta' a^2 q^2 + \eta_1' a^4)[(q^2 + l_1' a^2)(q^2 + l_2' a^2) + l_3' a^2]}{a^2[(q^2 + l_2' a^2)(q^2 - \lambda' a^2) + 2l_4' a^2]}, \tag{5.4}$$

where the additional terms for the cholesteric formulation, l_3' and l_4', are functions of $h^2\tau^2$, and

$$-l_3' \gg -l_4' > 0, \qquad \lambda' \gg 1, \tag{5.5}$$

for the values of the material parameters considered in this paper. One again deduces that the weak chirality reduces the magnitude of the critical Rayleigh number and the threshold, and to first order the dependence on $h\tau$ is quadratic.

Roll axis of arbitrary direction

When the direction of the roll axis is at an arbitrary angle in the (x, y) plane, it appears that the system of equations derived from Eq. (2.3)–(2.6) is such that the Fourier series method of solution cannot be used. An appropriate alternative method of solution is to integrate the system of equations directly by an orthonormalization procedure described by Barratt and Sloan.[17] However, we do not give details here for the following reasons. Firstly, a further description of this numerical procedure would make the present paper unduly long. Secondly, and more importantly, this method reveals that the minimum threshold gradient for a uniform parallel alignment, in fact, occurs when the roll axis is perpendicular to the initial orientation, at least for the values of the material parameters considered here. Lastly, this purely numerical approach provides no information regarding the analytic nature of the instability, in contrast to the Jeffries method.

In the latter vein, it follows from Eqs. (3.4), (3.5), (5.2), and (5.3) that the product ϕh^4 depends upon the wavenumber a and the product $\tau^2 h^2$. Consequently, at the critical threshold, ϕh^4 is some function of $\tau^2 h^2$ or equivalently h^2/P^2, but our numerical results are not sufficient to give a clear indication as to this dependence. In her approximate calculations Dubois-Voilette[5] finds that the threshold gradient ϕ is inversely proportional to the square of both the gap width h and the pitch P. Therefore, in our notation, she finds that ϕh^4 is directly proportional to the square of the product τh. However, since Dubois-Voilette considers large values for τh and we assume small values, there is no reason to anticipate that the functional dependence should be the same in these two limiting cases.

6. NUMERICAL RESULTS AND DISCUSSION

In order to obtain quantitative results by the Fourier series method, it is necessary to prescribe values for the various material parameters arising in the theory. In the absence of cholesteric data for all of the required parameters, and since cholesterics with sufficiently long pitch are produced by incorporating optically active additives in a sample of nematic liquid crystal, we follow other similar studies[5] and adopt the available mechanical data for a typical nematic liquid crystal, namely MBBA. The viscosities are taken to be those given by Gähwiller,[18] thermal conductivities and elastic constants as given by Dubois-Voilette[14] and Haller[19] respectively, and we take $\rho' g = -1 g cm^{-2} s^{-2} K^{-1}$.

Before listing the numerical results, we note two computational problems encountered in the solution. Firstly, it was necessary to use Richardson extrapolation to obtain accurate estimates for the sums of the slowly converging infinite series in Eq. (4.15) for $i = 1$ and $i = 2$. Secondly, to evaluate the determinant in Eq. (4.16) one uses the Crout decomposition with partial pivoting to reduce the growth of rounding errors.

Table I displays the computed values of the threshold gradient ϕ and its associated wavenumber a for several values of P/h and sample thicknesses of 1 mm and 0.5 mm for both planar and homeotropic alignments. The results for P/h infinite are in agreement with those of Dubois-Voilette[14] and Barratt and Sloan[13,17] for a nematic liquid crystal.

We make some observations on the results summarized in Table I. The first is that for both uniform alignments, the magnitude of the threshold gradient progressively decreases with the pitch P of the cholesteric sample. The reduction is relatively small over the values of P considered in this paper, being of the order of 3% for the homeotropic alignment and 7% for the uniform planar orientation. These results are qualitatively similar to those presented by Barratt and Sloan[17] for a twisted planar sample of nematic liquid crystal where the presence of an induced twist leads to a small reduction in the critical threshold gradient. It is interesting to note that when P assumes smaller values than those considered here, the magnitude of the threshold gradient continues to decrease more rapidly, although the assumed initial uniform alignments may no longer be valid. Finally, we note that the value of the non-dimensional wavenumber a for the critical threshold gradient does not change appreciably with P for each orientation.

From these calculations the addition of some chiral dopant to a nematic liquid crystal appears not to lead to any dramatic changes in these thermal

TABLE I

Threshold gradient $\phi\, K\, cm^{-1}$ and its associated non-dimensional wavenumber a for various values of P/h for both planar and homeotropic initial alignments.

	Planar alignment			Homeotropic alignment		
		$h = 1$ mm	$h = 0.5$ mm		$h = 1$ mm	$h = 0.5$ mm
P/h	a	ϕ	ϕ	a	ϕ	ϕ
4	0.96	−25.0	−401	0.90	47.5	760
8	0.97	−26.5	−423	0.90	48.5	776
16	0.97	−26.8	−429	0.91	48.7	779
∞	0.97	−26.9	−431	0.91	48.8	781

instabilities. It would be of general interest to verify these predictions experimentally, as it could conceivably be of interest in practical applications. Furthermore, experimental confirmation, or otherwise, of these theoretical predictions would yield useful information regarding the relevance of continuum theory to such problems. In particular, such comparisons would give an indication of the relative importance of the thermomechanical coupling terms omitted from this analysis.

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APPENDIX I

Here we define the coefficients which appear in Eq. (2.4) and (2.5):

$$2A_{ijkm} = 2\alpha_1 n_i n_j n_k n_m + (\alpha_2 + \alpha_5) n_j n_m \delta_{ik} + (\alpha_3 + \alpha_6) n_i n_j \delta_{km} + (\alpha_5 - \alpha_2) n_k n_m \delta_{ij} + \alpha_4 \delta_{ij} \delta_{km}$$

$$B_{ijk} = \alpha_2 n_k \delta_{ij} + \alpha_3 n_i \delta_{jk}$$

$$C_{ijkm} = (K_1 - K_2)\delta_{im}\delta_{jk} + (K_3 - K_2) n_k n_m \delta_{ij} + K_2 \delta_{ij}\delta_{km}$$

$$2D_{ijk} = (\gamma_1 - \gamma_2) n_k \delta_{ij} - (\gamma_1 + \gamma_2) n_j \delta_{ik}$$

and

$$\gamma_1 = \alpha_3 - \alpha_2, \qquad \gamma_2 = \alpha_6 - \alpha_5 .$$

Our notations are those of Leslie.[3]

APPENDIX II

For the homeotropic alignment, the coefficients in Eq. (3.4) and (3.5) take the values

$$\kappa = \frac{\kappa_1}{\kappa_1 + \kappa_2}, \qquad \eta = \frac{2\alpha_1 + \eta_a + \eta_b}{\eta_a}, \qquad \eta_a = \alpha_4 + \alpha_5 - \alpha_2$$

$$\eta_b = \alpha_3 + \alpha_4 + \alpha_6, \qquad \eta_1 = \frac{\eta_b}{\eta_a}, \qquad l_1 = \frac{K_1}{K_3}, \qquad l_2 = \frac{K_2}{K_3}$$

$$l_3 = \frac{4K_2^2\tau^2h^2}{\pi^2K_3^2}, \qquad l_4 = \frac{4CK_2^2\tau^2h^2}{\pi^2K_3[(\gamma_1 - \gamma_2)\kappa_2 + 2CK_3]}$$

$$\lambda = \frac{-(\gamma_1 + \gamma_2)\kappa_2 - 2CK_1}{(\gamma_1 - \gamma_2)\kappa_2 + 2CK_3}, \qquad R = \frac{-\rho' g\phi[(\gamma_1 - \gamma_2)\kappa_2 + 2CK_3]h^4}{\pi^4(\kappa_1 + \kappa_2)\eta_a K_3}$$

For the initial planar alignment the coefficients in Eq. (5.2) and (5.3) take the values

$$\kappa' = \frac{1}{\kappa} \qquad \eta' = \frac{\eta}{\eta_1}, \qquad \eta_1' = \frac{1}{\eta_1}, \qquad l_1' = \frac{1}{l_1}, \qquad l_2' = \frac{1}{l_2}$$

$$l_3' = \frac{-4K_2\tau^2h^2}{K_1\pi^2}, \qquad l_4' = \frac{-4CK_2\tau^2h^2}{\pi^2[-(\gamma_1 + \gamma_2)\kappa_2 + 2CK_1]}$$

$$\lambda' = \frac{(\gamma_1 - \gamma_2)\kappa_2 - 2CK_3}{-(\gamma_1 + \gamma_2)\kappa_2 + 2CK_1}, \qquad R' = \frac{-\rho' g\phi[-(\gamma_1 + \gamma_2)\kappa_2 + 2CK_1]h^4}{\pi^4\kappa_1\eta_b K_1}$$

The constants γ_1 and γ_2 are defined in Appendix I.

APPENDIX III

Here we define the Q_1, Q_2, Q_3, Q_4, Q_5 and the elements of the (5×5) matrices Φ and Ψ appearing in Sec. 4 for the initial homeotropic alignment.

$$Q_1 = (\eta + \kappa + l_1 + l_2)a^2 - l_3$$

$$Q_2 = (\eta + \kappa)(l_1a^2 + l_2a^2 - l_3)a^2 + (\eta_1 + \eta\kappa)a^4 + l_1l_2a^4$$

$$Q_3 = (\eta + \kappa)l_1l_2a^6 + (\eta_1 + \eta\kappa)(l_1a^2 + l_2a^2 - l_3)a^4 + \eta_1\kappa a^6 - Ra^2$$

$$Q_4 = (\eta_1 + \eta\kappa)l_1l_2a^8 + \eta_1\kappa(l_1a^2 + l_2a^2 - l_3)a^6 + R[(\lambda - l_2)a^2 + 2l_4]a^2$$

$$Q_5 = \eta_1\kappa l_1l_2a^{10} + R\lambda l_2a^6$$

$$\Phi_{1_j} = \frac{1}{(2j-2)!}\left(\frac{\pi}{2}\right)^{2j-2}, \qquad j = 1, 2, \ldots, 5$$

$$\Phi_{21} = 0, \qquad \Phi_{2_j} = \frac{1}{(2j-3)!}\left(\frac{\pi}{2}\right)^{2j-3}, \qquad j = 2, 3, \ldots, 5$$

$$\Phi_{31} = 0, \qquad \Phi_{32} = -\eta a^2, \qquad \Phi_{3_j} = \frac{1}{(2j-6)!}\left(\frac{\pi}{2}\right)^{2j-6} - \frac{\eta a^2}{(2j-4)!} \cdot \left(\frac{\pi}{2}\right)^{2j-4}, \qquad j = 3, 4, 5$$

$$\Phi_{41} = 0, \qquad \Phi_{42} = \eta_1 a^4, \qquad \Phi_{43} = -\eta a^2 + \frac{\eta_1 a^4}{2!}\left(\frac{\pi}{2}\right)^2$$

$$\Phi_{4_j} = \frac{1}{(2j-8)!}\left(\frac{\pi}{2}\right)^{2j-8} - \frac{\eta a^2}{(2j-6)!}\left(\frac{\pi}{2}\right)^{2j-6} + \frac{\eta_1 a^4}{(2j-4)!} \cdot \left(\frac{\pi}{2}\right)^{2j-4}, \qquad j = 4, 5$$

$$\Phi_{51} = \Phi_{52} = 0, \qquad \Phi_{53} = c_3\left(\frac{\pi}{2}\right), \qquad \Phi_{54} = -c_2\left(\frac{\pi}{2}\right) + \frac{c_3}{3!}\left(\frac{\pi}{2}\right)^3$$

$$\Phi_{55} = c_1\left(\frac{\pi}{2}\right) - \frac{c_2}{3!}\left(\frac{\pi}{2}\right)^3 + \frac{c_3}{5!}\left(\frac{\pi}{2}\right)^5$$

$$c_1 = (\eta + \kappa + l_1)a^2 - l_3, \qquad c_2 = [\eta_1 + \kappa l_1 + \eta(\kappa + l_1)]a^4 - (\eta + \kappa)l_3a^2$$

$$c_3 = [\eta_1(\kappa + l_1) + \eta\kappa l_1]a^6 - (\eta_1 + \eta\kappa)l_3a^4 - Ra^2$$

$$\Psi_{25} = 1, \qquad \Psi_{51} = -1, \qquad \Psi_{52} = -c_1, \qquad \Psi_{53} = -c_2, \qquad \Psi_{54} = -c_3$$

otherwise

$$\Psi_{ij} = 0.$$

The corresponding values for the initial planar alignment are

$$Q_1' = (\eta' + \kappa' + l_1' + l_2')a^2$$

$$Q_2' = (\eta' + \kappa')(l_1' + l_2')a^4 + (\eta_1' + \eta'\kappa')a^4 + (l_1'l_2'a^2 + l_3')a^2$$

$$Q_3' = (\eta' + \kappa')(l_1'l_2'a^2 + l_3')a^4 + (\eta_1' + \eta'\kappa')(l_1' + l_2')a^6 + \eta_1'\kappa'a^6 - R'a^2$$

$$Q_4' = (\eta_1' + \eta'\kappa')(l_1'l_2'a^2 + l_3')a^6 + \eta_1'\kappa'(l_1' + l_2')a^8 + (\lambda' - l_2')R'a^4$$

$$Q_5' = \eta_1'\kappa'(l_1'l_2'a^2 + l_3')a^8 - (2l_4' - l_2'\lambda'a^2)R'a^4$$

$$\Phi_{1_j}' = \frac{1}{(2j-2)!}\left(\frac{\pi}{2}\right)^{2j-2}, \qquad j = 1, 2, \ldots, 5$$

$$\Phi_{21}' = 0, \qquad \Phi_{2_j}' = \frac{1}{(2j-3)!}\left(\frac{\pi}{2}\right)^{2j-3}, \qquad j = 2, 3, \ldots, 5$$

$$\Phi_{31}' = 0, \qquad \Phi_{32}' = -\eta'a^2, \qquad \Phi_{3_j}' = \frac{1}{(2j-6)!}\left(\frac{\pi}{2}\right)^{2j-6} - \frac{\eta'a^2}{(2j-4)!} \cdot \left(\frac{\pi}{2}\right)^{2j-4}, \qquad j = 3, 4, 5$$

$$\Phi_{41}' = 0, \qquad \Phi_{42}' = \eta_1'a^4, \qquad \Phi_{43}' = -\eta'a^2 + \frac{\eta_1'a^4}{2!}\left(\frac{\pi}{2}\right)^2$$

$$\Phi_{4_j}' = \frac{1}{(2j-8)!}\left(\frac{\pi}{2}\right)^{2j-8} - \frac{\eta'a^2}{(2j-6)!}\left(\frac{\pi}{2}\right)^{2j-6} + \frac{\eta_1'a^4}{(2j-4)!} \cdot \left(\frac{\pi}{2}\right)^{2j-4}, \qquad j = 4, 5$$

$$\Phi_{51}' = 0, \qquad \Phi_{52}' = R'a^2, \qquad \Phi_{53}' = \eta_1'a^4 + \frac{R'a^2}{2!}\left(\frac{\pi}{2}\right)^2$$

$$\Phi_{54}' = -\eta'a^2 + \frac{\eta_1'a^4}{2!}\left(\frac{\pi}{2}\right)^2 + \frac{R'a^2}{4!}\left(\frac{\pi}{2}\right)^4$$

$$\Phi_{55}' = 1 - \frac{\eta'a^2}{2!}\left(\frac{\pi}{2}\right)^2 + \frac{\eta_1'a^4}{4!}\left(\frac{\pi}{2}\right)^4 + \frac{R'a^2}{6!}\left(\frac{\pi}{2}\right)^6$$

$$\Psi_{25}' = 1$$

otherwise

$$\Psi_{ij}' = 0$$