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CYLINDRICAL, SPHERICAL AND TOROIDAL LAYERING OF SMECTIC C LIQUID CRYSTALS

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Cylindrical, Spherical and Toroidal Layering of Smectic C Liquid Crystals

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This article examines static solutions to the smectic C continuum equations of Leslie *et al.*[1] for a variety of layer geometries. In particular it is shown that valid molecular configurations exist for cylindrical, spherical and toroidal layers. Suitable parameterizations are introduced for each surface and the Euler-Lagrange balance equations are solved in a suitable coordinate system. Plots of the surfaces are presented, and their relationship to singularities in the solutions are discussed.

Keywords: smectic C liquid crystals; continuum theory; static solutions

INTRODUCTION

The isothermal smectic C continuum theory proposed by Leslie *et al.*[1] has proved useful for mathematical analyses of both static and dynamic problems in a number of different geometries.[2-7] The theory is based on two simple assumptions, the smectic layers, although deformed, remain of constant thickness, and also the angle of tilt of the alignment with respect to the layer normal remains fixed. A serious test for any such static theory of smectics is that it must predict layers forming complex surfaces such as Dupin or parabolic cyclides.[8,9] Static solutions for such layered structures have been verified using the static theory,[2,4] although these solutions are often restricted by constraints on the elastic constants of the materials.

Although mentioned in previous articles, no solutions have been detailed for cylindrical, spherical or toroidal layers. The aim of this article is to present valid molecular configurations for each of these types of layering. In each case we will outline the method of solution and discuss any problems which arise due to singularities or

line defects. Cecil[10] and Stewart and McKay[11] discuss the mathematical relationship between the Dupin and parabolic cyclides and the geometries examined here. However it is worth noting that the parameterization of a torus may be derived from that of a Dupin cyclide if the eccentricity of the underlying focal domain reduces to zero.

In the following Sections we introduce the smectic C continuum theory of Leslie *et al.*[1] In particular we discuss the Euler-Lagrange static equilibrium equations and the associated Lagrange multipliers. We examine solutions for, respectively, cylindrical, spherical and toroidal layered structures; in each case we introduce a suitable parameterization for the surfaces before examining one molecular configuration. Details and calculations for a second valid solution for each layering are given in Stewart and McKay.[11]

SMECTIC CONTINUUM THEORY

Liquid crystals are elongated molecules for which the long molecular axes locally adopt one common direction in space, usually described by a unit vector $\boldsymbol{n}$, known as the director. Smectic C liquid crystals are layered structures where the director makes an angle θ with respect to the layer normal. The smectic structure can be described via a pair of orthogonal unit vectors $\boldsymbol{a}$ and $\boldsymbol{c}$. Vector $\boldsymbol{a}$ is the density wave vector which also coincides with the smectic layer normal due to the constant thickness assumption. Away from dislocations we must have[12]

$$\nabla \times \boldsymbol{a} = \boldsymbol{0}. \tag{1}$$

The unit vector $\boldsymbol{c}$ is the unit orthogonal projection of $\boldsymbol{n}$ onto the smectic planes. Thus $\boldsymbol{c}$ is always tangential to the smectic layers. It follows that the directors $\boldsymbol{a}$ and $\boldsymbol{c}$ must be subject to the constraints

$$\boldsymbol{a} \cdot \boldsymbol{a} = \boldsymbol{c} \cdot \boldsymbol{c} = 1, \qquad \boldsymbol{a} \cdot \boldsymbol{c} = 0. \tag{2}$$

A bulk energy for the sample, W, can be constructed based on $\boldsymbol{a}$, $\boldsymbol{c}$ and their gradients:

$$\begin{aligned} 2W = {} & K_1(\nabla \cdot \boldsymbol{a})^2 + K_2(\nabla \cdot \boldsymbol{c})^2 + K_3(\boldsymbol{a} \cdot \nabla \times \boldsymbol{c})^2 \\ & + K_4(\boldsymbol{c} \cdot \nabla \times \boldsymbol{c})^2 + K_5(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c})^2 + 2K_6(\nabla \cdot \boldsymbol{a})(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c}) \\ & + 2K_7(\boldsymbol{a} \cdot \nabla \times \boldsymbol{c})(\boldsymbol{c} \cdot \nabla \times \boldsymbol{c}) + 2K_8(\nabla \cdot \boldsymbol{c})(\boldsymbol{b} \cdot \nabla \times \boldsymbol{c}) \\ & + 2K_9(\nabla \cdot \boldsymbol{a})(\nabla \cdot \boldsymbol{c}), \end{aligned} \tag{3}$$

where the K_i's are elastic constants and unit vector $\boldsymbol{b} = \boldsymbol{a} \times \boldsymbol{c}$. The relationship between these elastic constants and those of the Orsay Group[13] is described in Leslie *et al.*[14]

In the absence of body forces the Euler-Lagrange static equilibrium equations are[1]

$$\boldsymbol{\Pi}^{\boldsymbol{a}} + \gamma \boldsymbol{a} + \mu \boldsymbol{c} + \nabla \times \boldsymbol{\beta} = 0, \tag{4}$$

$$\boldsymbol{\Pi}^{\boldsymbol{c}} + \tau \boldsymbol{c} + \mu \boldsymbol{a} = 0, \tag{5}$$

where γ, μ, τ and $\boldsymbol{\beta}$ are Lagrange multipliers which arise from the four constraints (1) and (2). The director body forces, $\boldsymbol{\Pi}^{\boldsymbol{a}}$ and $\boldsymbol{\Pi}^{\boldsymbol{c}}$, are

$$\Pi_i^a = \left(\frac{\partial W}{\partial (a_{i,j})}\right)_{,j} - \frac{\partial W}{\partial a_i}, \qquad \Pi_i^c = \left(\frac{\partial W}{\partial (c_{i,j})}\right)_{,j} - \frac{\partial W}{\partial c_i},$$

where, for example, $a_{i,j}$ denotes partial differentiation of the ith component of $\boldsymbol{a}$ with respect to the jth variable and repeated indices follow the summation convention. Vector forms for $\boldsymbol{\Pi}^{\boldsymbol{a}}$ and $\boldsymbol{\Pi}^{\boldsymbol{c}}$ may be found in Nakagawa.[2]

Employing (2), (4) and (5), we can calculate the Lagrange multipliers μ and τ via appropriate scalar products,

$$\mu = -\boldsymbol{\Pi}^{\boldsymbol{c}} \cdot \boldsymbol{a}, \qquad \tau = -\boldsymbol{\Pi}^{\boldsymbol{c}} \cdot \boldsymbol{c}. \tag{6}$$

In the following sections we will propose solutions to (4), (5) for a variety of layer geometries. For any molecular configuration to be valid it must automatically satisfy constraints (1), (2), and from (5),

$$\boldsymbol{\Pi}^{\boldsymbol{c}} \cdot \boldsymbol{b} = 0. \tag{7}$$

We also require to find the Lagrange multipliers via (4) and (6), in particular γ and $\boldsymbol{\beta}$. The former is calculated by taking the divergence of (4), eliminating $\boldsymbol{\beta}$ in the process. Finally, (4) is integrated in order to solve for $\boldsymbol{\beta}$. In each case we need to ensure that the multipliers are free from singularities on the smectic layer, except possibly on line defects associated with the layer.

CYLINDRICAL LAYERING

Figure 1(a) describes a single cylindrical layer of radius r. Varying r provides a family of concentric infinite cylinders sharing a common

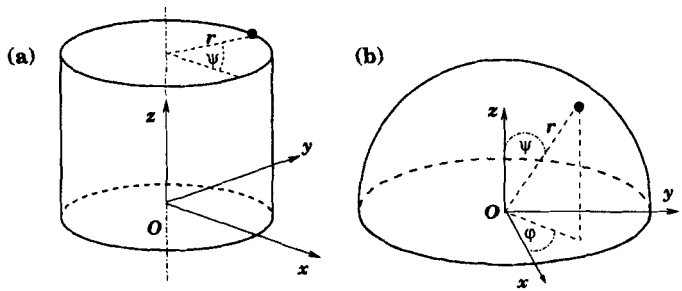

FIGURE 1. Description of coordinate systems for (a) cylindrical and (b) spherical layers

centre axis, equidistant if r changes by the same amount, e.g. $r = 1, 2, 3, \ldots$, etc. We can fully describe this series of cylinders by parameterizing,

$$x = r\cos\psi, \qquad y = r\sin\psi, \qquad z = z,$$

where $r > 0$, $0 \leq \psi \leq 2\pi$, $z \in \mathbb{R}$. In the following analysis, all vectors are expressed in terms of the new (r, ψ, z) coordinate system. The normal to any cylindrical surface is therefore given by $\boldsymbol{a} = \operatorname{grad} r = (1, 0, 0)$.

Consider the case when $\boldsymbol{a} = (1, 0, 0)$, $\boldsymbol{c} = (0, 0, 1)$ and $\boldsymbol{b} = (0, -1, 0)$. In this molecular configuration the projection director $\boldsymbol{c}$ is in the direction of the cylindrical axis. Following the notation introduced previously it can be shown that

$$\boldsymbol{\Pi}^{a} = -\frac{K_1}{r^2}\boldsymbol{a}, \qquad \boldsymbol{\Pi}^{c} = -\frac{K_9}{r^2}\boldsymbol{a}.$$

Subsequently it is straightforward to derive the four Euler-Lagrange multipliers,

$$\mu = \frac{K_9}{r^2}, \qquad \tau = 0, \qquad \gamma = \frac{K_1}{r^2}, \qquad \boldsymbol{\beta} = K_9\frac{\ln r}{r}\boldsymbol{b}.$$

(Singularities at $r = 0$ may be ignored as they coincide with the central axis of the cylinder.) Therefore we have shown that our solution satisfies the balance equations and constraints (1)–(5).

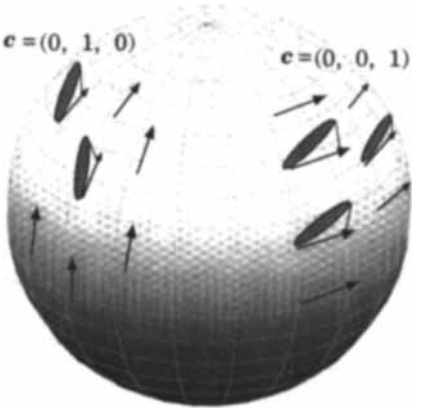

FIGURE 2. Molecule configuration for spherical geometry. Arrows indicate direction of $\boldsymbol{c}$ in either the ψ-direction, $\boldsymbol{c} = (0, 1, 0)$, or in the ϕ-direction, $\boldsymbol{c} = (0, 0, 1)$

SPHERICAL LAYERING

A family of concentric spheres, see Figure 1(b), can be described via the parameterization

$$x = r\sin\psi\cos\phi, \qquad y = r\sin\psi\sin\phi, \qquad z = r\cos\psi,$$

where $r > 0$, $0 \leq \psi, \phi \leq 2\pi$. Once we transform to the (r, ψ, ϕ) system, the outward normal to any surface is again $\boldsymbol{a} = \operatorname{grad} r = (1, 0, 0)$. Although Leslie *et al.*[1] state that static solutions can be found for a spherical layering, ignoring singularities, no details of the calculations are specified.

A solution is easily obtained[11] when molecules lie in the polar ψ-direction, i.e. $\boldsymbol{c} = (0, 1, 0)$. Here we concentrate on the ϕ-direction, $\boldsymbol{c} = (0, 0, 1)$, also shown in Figure 2. In this case the director forces correspond to

$$\begin{aligned}\boldsymbol{\Pi}^{\boldsymbol{a}} &= -(2K_1 - K_3 + K_5 + 3K_6)\frac{1}{r^2}\boldsymbol{a} + K_7\frac{1}{r^2\sin^2\psi}\boldsymbol{c} \\ &\quad -(K_3 - K_5 - 2K_6)\frac{1}{r^2\tan\psi}\boldsymbol{b}, \\ \boldsymbol{\Pi}^{\boldsymbol{c}} &= (2K_7 - K_8 - 2K_9)\frac{1}{r^2}\boldsymbol{a} - (2K_3 - K_4)\frac{1}{r^2\sin^2\psi}\boldsymbol{c}\end{aligned}$$

$$+2(K_3 - K_5 - 2K_6)\frac{1}{r^2}\boldsymbol{c} - K_7\frac{1}{r^2\tan\psi}\boldsymbol{b}.$$

Immediately we can deduce that $\boldsymbol{\Pi}^{\mathbf{c}}$ does not satisfy criteria (7) for a solution to exist for all nine terms in the energy. The configuration we consider will satisfy the balance equations only for a material for which the elastic constant $K_7 \equiv 0$. For example, materials which exhibit the smectic C_M phase (see Brand and Pleiner[15]) have a six term energy given by the first six terms in (3). With this constraint we can assign Lagrange multipliers which allow us to satisfy the balance equations:

$$\begin{aligned}
\tau &= (2K_3 - K_4)\frac{1}{r^2\sin^2\psi} - 2(K_3 - K_5 - 2K_6)\frac{1}{r^2}, \\
\mu &= (K_8 + 2K_9)\frac{1}{r^2}, \\
\gamma &= (2K_1 - K_3 + K_5 + 3K_6)\frac{1}{r^2} + (K_3 - K_5 - 2K_6)\frac{\ln r}{r^2}, \\
\boldsymbol{\beta} &= (K_8 + 2K_9)\frac{\ln r}{r}\boldsymbol{b} + (K_3 - K_5 - 2K_6)\frac{\ln r}{r\tan\psi}\boldsymbol{c}.
\end{aligned}$$

As expected these multipliers exhibit singularities on the line defect corresponding to $\psi = 0$ where the molecules converge at the top and bottom of the sphere. However the configuration under consideration will satisfy the balance equations on the remainder of any uniaxial spherical layering.

TOROIDAL LAYERING

A torus is the limiting example of the Dupin (or hyperbolic) cyclide, a taut, compact, two-dimensional surface (see Leslie *et al.*[4] and references therein). These surfaces can be layered over each other to form parallel equidistant layered structures. Previously, Nakagawa[2] and Leslie *et al.*[1] examined one possible static solution of the smectic equations for a Dupin cyclide, subject to certain constraints on the elastic constants. Although they show that it may be possible to find a solution, they do not calculate the individual Lagrange multipliers. In particular they do not consider the intricacies involved in guaranteeing that the multipliers are defined on the whole cyclide. Here we introduce another possible configuration not previously discussed. We outline the problems involved in obtaining

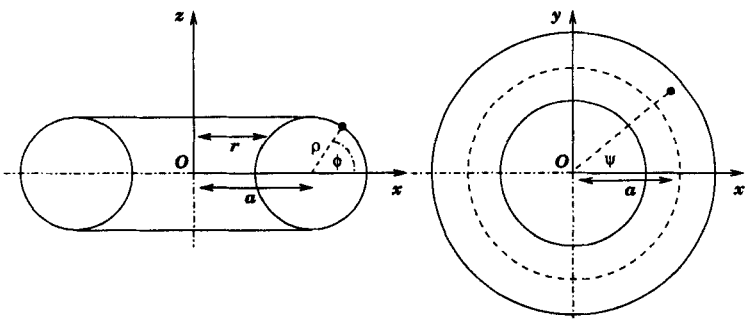

FIGURE 3. Geometrical representation of toroidal surface

valid multipliers, in particular γ and $\boldsymbol{\beta}$, and discuss any restrictions necessary on the elastic constants.

The torus shown in Figure 3 may be described via

$$\rho^2 = (r-a)^2 + z^2, \qquad x^2 + y^2 = r^2,$$

where a is the internal radius of the torus and ρ is the outer radius as indicated. A family of layered tori may be constructed by varying ρ for fixed a. The toroidal surface can now be parameterized,

$$x = (a + \rho\cos\phi)\cos\psi, \qquad y = (a + \rho\cos\phi)\sin\psi, \qquad z = \rho\sin\phi, \tag{8}$$

where

$$r(\rho, \phi) = a + \rho\cos\phi, \qquad 0 < \rho < a, \qquad 0 \le \psi, \phi \le 2\pi.$$

Here ψ is the internal polar angle while ϕ is the external polar angle. In the calculations which follow we utilize the orthogonal (ρ, ψ, ϕ) coordinate system. The parameterization (8) is equivalent to the reduction of Forsyth's[16] representation of the Dupin cyclide. Nakagawa[2] employs a different parameterization of the cyclide which describes only the inner portion of the surface. We shall see later that this approach omits points on the torus which have an important bearing on the validity of solutions.

When the molecules are aligned in the polar ψ-direction, $\boldsymbol{c} = (0, 1, 0)$, as shown in Figure 4, the solution is analagous to that for the Dupin cyclide discussed in Nakagawa.[2] Due to the constraint (7), for our solution to exist we must restrict our elastic constants such that $K_7 = 0$ and $K_8 + K_9 = 0$. Furthermore, γ and $\boldsymbol{\beta}$ must be

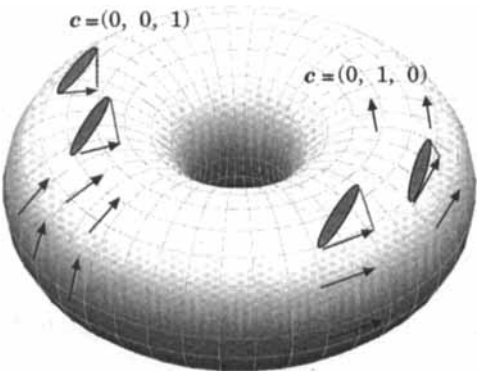

FIGURE 4. Molecule configuration when $\boldsymbol{c}$-director points in the ψ-direction, $\boldsymbol{c} = (0, 1, 0)$, or in the ϕ-direction, $\boldsymbol{c} = (0, 0, 1)$.

chosen carefully to ensure that they are defined on the whole torus, excluding possibly the central axis defect corresponding to $r = 0$.

We now consider an alternative setup, not previously discussed, where the molecules traverse the torus in the ϕ-direction, $\boldsymbol{c} = (0, 0, 1)$, also indicated in Figure 4. Substituting the proposed configuration into (4) and (6), we derive the following multipliers (details of the balance forces, which have no $\boldsymbol{b}$-components, have been omitted),

$$\begin{aligned}
\tau &= K_2 \frac{1}{\rho^2 r^2}\left(a(r-a)+\rho^2\right) + K_4\,\frac{a-2r}{r\rho^2} + K_5\frac{2}{\rho^2} + K_6\frac{2(2r-a)}{r\rho^2} \\
&\quad + (K_7 - K_8)\,\frac{2\sin\phi}{r\rho} + K_9\,\frac{a\sin\phi}{\rho r^2}, \\
\mu &= -K_2\frac{\sin\phi\cos\phi}{r^2} - K_3\,\frac{\sin\phi}{r\rho} - K_7\,\frac{(2r-a)}{r\rho^2} + K_8\,\frac{1}{\rho^2} \\
&\quad + K_9\left(\frac{a^2 - 2r(a-r)}{r^2\rho^2}\right), \\
\gamma &= -K_1\left(\frac{2r(a-r)-a^2}{r^2\rho^2}\right) + (K_5 - K_3)\frac{1}{\rho^2} + K_6\left(\frac{1}{\rho^2} + \frac{2r-a}{r\rho^2}\right) \\
&\quad + (K_7 - K_8)\,\frac{\sin\phi}{r\rho} - K_9\,\frac{\sin\phi\cos\phi}{r^2} + \hat{\gamma}.
\end{aligned}$$

The resulting balance equation for the smectic sample may now be

rewritten as

$$\operatorname{curl}\boldsymbol{\beta}+\hat{\gamma}\boldsymbol{a} = \left\{A_1\frac{a\sin\phi}{r^2\rho}+A_2\frac{\sin\phi}{r\rho}+A_3\frac{a}{r\rho^2}+K_9\frac{1-2\cos^2\phi}{r^2}\right\}\boldsymbol{c},$$

where

$$A_1 = K_1 - K_2, \qquad A_2 = K_2 + K_5 + 2K_6, \qquad A_3 = -K_8 - K_9.$$

Following the procedure outlined previously, we can evaluate multipliers $\hat{\gamma}$ and $\boldsymbol{\beta}$,

$$\begin{aligned}\hat{\gamma}(\rho,\phi) &= A_1\left(\frac{\cos\phi}{r\rho}\ln\left(\frac{\rho}{r}\right)+\frac{\sin^2\phi}{r^2}\right)+A_2\frac{\cos\phi}{r\rho}\ln\rho \\ &\quad +K_9\frac{\sin\phi}{r^2\rho\cos^2\phi}\Big(\,(1+2\cos^2\phi)r\ln r + a(1-2\cos^2\phi)\,\Big),\end{aligned}$$

$$\begin{aligned}\boldsymbol{\beta} &= \Bigg[-A_1\frac{\sin\phi}{r}\ln\left(\frac{\rho}{r}\right)-A_2\frac{\sin\phi}{r}\ln\rho+A_3\frac{a}{r\rho} \\ &\quad + K_9\Big(\frac{1-2\cos^2\phi}{r\cos\phi}\ln r+\frac{1+\cos^2\phi}{\cos\phi}\Big)\Bigg]\boldsymbol{b}.\end{aligned}$$

There remains a problem with the K_9 term in $\hat{\gamma}$ and $\boldsymbol{\beta}$; in both cases the multipliers diverge as ϕ approaches $\frac{\pi}{2}$ or $\frac{3\pi}{2}$. These singularities correspond to circles at the extreme top and bottom of the toroidal surface. (These lines may be denoted alternatively as $r \equiv a$.) It is not possible to remove these singularities when calculating $\hat{\gamma}$ and $\boldsymbol{\beta}$; therefore the proposed solution to the balance equations exists only for a material for which $K_9 \equiv 0$. Alternatively the configuration is valid for a full nine term bulk energy for a partial torus surface. Leslie *et al.*[3] encounter a similar problem in their study of smectic solutions for the parabolic cyclide and therefore restrict their attention to the six term energy of smectic C_M or anti-ferroelectric smectic phases.

Note that the parameterization of Nakagawa[2] describes only the inner portion of the torus. It can be easily adapted to parameterize the outer section of the surface. However, unlike the reduction of Forsyth's[16] Dupin cyclide parameterization, the description in Nakagawa[2] always excludes the circles corresponding to $\phi = \frac{\pi}{2}, \frac{3\pi}{2}$, and as a result does not consider the problems associated with calculating the multipliers on these lines.

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