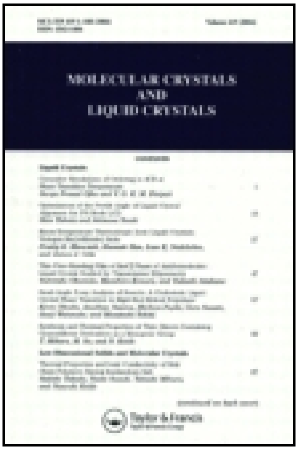

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Average Orientation in a Three-Dimensional Layer of Nematic Liquid Crystal

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The average orientation of a nematic liquid crystal is calculated from the Ericksen–Leslie theory for a three-dimensional parallelepiped. When strong magnetic, electric or flow fields are present to determine the orientation, existing results show the effect of side walls on orientation is not great. In the absence of these forces, however, the side walls can influence the average orientation in the sample, e.g. when the homeotropic orientation of a side wall causes an orientation perpendicular to the homeotropic orientation of the top and bottom surfaces. Calculations give the average orientation when only surface effects are considered, i.e. in the absence of magnetic, electric and flow fields, for a homeotropic orientation of the liquid crystal on all surfaces. Results are well approximated by

$$\overline{\cos^2 \phi} = 1 - (2/3)(L_z/L_x)$$

where the overbar denotes a transverse average (in the x and y directions), ϕ is the angle between the vertical z axis and the director, L_z is the thickness of the layer, and L_x is the length of the side of a square layer.

Nematic liquid crystals display an anisotropy in many of their properties such as thermal and electrical conductivity, dielectric constant and diffusivity. When these properties are measured across a macroscopic sample, the orientation of the director may vary throughout the sample and the measured properties depend on an average in some sense over the volume of the sample. When a magnetic field H is applied, the coherence length ξ is determined by de Gennes,[1] $\xi H = (k/\Delta\chi)^{1/2}$, where k is an elastic constant and $\Delta\chi$ is the volume magnetic susceptibility. For a moderate H the orientation of the sample is constant in space, except for thin layers near the boundaries. The average orientation is then determined by the orientation of H. When flow

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occurs, or both flow and a magnetic field are present, Finlayson's[2] results can be used to assess the relative importance of the orientation specified at the wall. Thus criteria exist to determine when the average orientation of a sample is essentially the constant orientation, except near the walls.

When no external orienting forces are present, though, the only forces controlling the orientation are surface and elastic forces. In a one-dimensional case, say between two flat plates of infinite extent, the surface orientation holds throughout the same (if the boundary conditions of the two surfaces are compatible). However, samples are not infinite in extent, and the question arises as to how thin a sample must be for the side walls to have a negligible effect on the average orientation. Calculations are reported below to answer this question for homeotropic orientation on all surfaces (top, bottom, and sides) of three-dimensional parallelepipeds.

The three-dimensional director equation in the absence of flow or external fields is obtained from the Ericksen–Leslie theory.[2] The vector product of the director and the director equation gives

$$\gamma_1 \mathbf{n} x \frac{\partial \mathbf{n}}{\partial t} = k_{22} \mathbf{n} x (\nabla^2 \mathbf{n}) + (k_{11} - k_{22}) \mathbf{n} x \nabla (\nabla \cdot \mathbf{n}) + (k_{33} - k_{22}) \mathbf{n} x [\nabla \cdot (\mathbf{nn} \cdot \nabla \mathbf{n}) - \nabla \mathbf{n} \cdot (\mathbf{n} \cdot \nabla \mathbf{n})] \tag{1}$$

This equation is solved under steady state conditions using the expanded equations presented in the Appendix.

An attending set of boundary conditions is obtained for the geometry shown in Figure 1. We make the director perpendicular to each boundary by setting $\phi = \pi/2$ and $\theta = 0$ at $x' = \pm 1$ ($x' = 2x/L_x$, $y' = 2y/L_y$, $z' = 2z/L_z$), $\phi = \pi/2$ and $\theta = \pi/2$ at $y' = \pm 1$, and $\phi = 0$ at $z' = \pm 1$. The symmetry of the problem allows solution in only one octant of the parallelepiped, with bilateral symmetry across the planes $x' = 0$, $y' = 0$, and $z' = 0$, as indicated in the Appendix.

The coupled set of differential equations, Eq. (4), are solved using the orthogonal collocation method using polynomials even in x', y', and z'.[1]

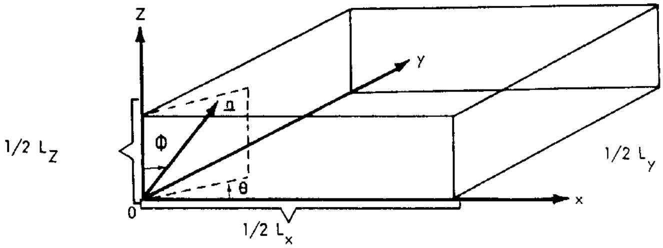

FIGURE 1 Coordinate system shown in relation to an octant of the 3-dimensional layer.

This method requires the differential equations to be satisfied at a set of grid or collocation points and converts the set of two partial differential equations to a set of $2(N + 1)^3$ algebraic equations, where N is the number of collocation points in each of the three directions interior to the octant.

The algebraic equations are solved by relaxation, in which the values of ϕ and θ are simultaneously recomputed at successive grid points while holding the values at other grid points constant. The computation of ϕ and θ from the nonlinear equations is accomplished by a bivariate Newton-Raphson iteration modified[3] to limit the changes in ϕ and θ.

Conduction-like transport properties can be represented by a conductivity tensor of the form

$$\boldsymbol{\sigma} = \sigma_t \boldsymbol{\delta} + (\sigma_a - \sigma_t)\mathbf{nn},$$

where $\boldsymbol{\sigma}$ is the conductivity tensor, σ_t is the conductivity measured perpendicular to $\mathbf{n}$, σ_a is the conductivity measured parallel to $\mathbf{n}$, and $\boldsymbol{\delta}$ is the second-rank tensor. The conductivity of a layer is given by

$$\frac{1}{\sigma} = \int_0^1 \frac{\mathrm{d}z'}{\sigma_t + (\sigma_a - \sigma_t)\int_0^1\int_0^1 \cos^2\phi(x', y', z')\mathrm{d}x'\,\mathrm{d}y'}$$

When ϕ is not constant we measure σ, an apparent conductivity. If we take $\overline{\cos^2\phi}$ as the value of $\cos^2\phi$ assuming ϕ is constant for that apparent conductivity, we get

$$\overline{\cos^2\phi} = \frac{1}{\sigma'}\left\{\frac{1}{\displaystyle\int_0^1 \frac{\mathrm{d}z'}{1 + \sigma'\int_0^1\int_0^1 \cos^2\phi(x', y', z')\mathrm{d}x'\,\mathrm{d}y'}} - 1\right\} \tag{2}$$

where $\sigma' = (\sigma_a - \sigma_t)/\sigma_t$. For the case $|\sigma_a - \sigma_t| \ll \sigma_t$ then the apparent conductivity measured in the z-direction is approximated by

$$\sigma_{\text{apparent}} = \sigma_t + (\sigma_a - \sigma_t)\overline{\cos^2\phi},$$

where

$$\overline{\cos^2\phi} = \int_0^1\int_0^1\int_0^1 \cos^2\phi(x', y', z')\mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}z'.$$

Values of $\overline{\cos^2\phi}$ are obtained as a function of L_z/L_x and presented in Figure 2 for various orders of approximation. $N = 4$ is sufficiently accurate for most purposes. The results are well approximated by

$$\overline{\cos^2\phi} = 1 - (2/3)(L_z/L_x) \tag{3}$$

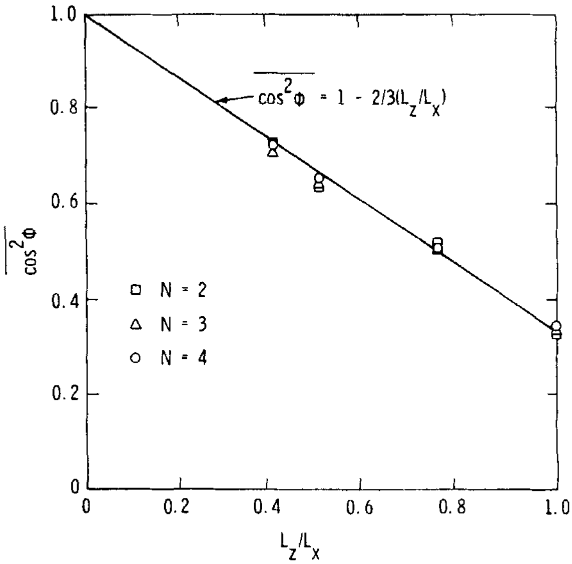

FIGURE 2 Computed values of $\overline{\cos^2 \phi}$ versus L_z/L_x for various orders of approximation, N.

which is found to be a linear interpolation between the two extremes

$$\lim_{L_z/L_x \to 0} \overline{\cos^2 \phi} = 1 \qquad \text{for a plane of infinite extent,}$$

and

$$L_z/L_x = 1, \overline{\cos^2 \phi} = \tfrac{1}{3} \qquad \text{for a cube.}$$

Notice that for a cubic specimen the apparent orientation is indistinguishable from that found if **n** varies randomly everywhere.

Equation (3) serves as a "rule of thumb" to determine the width-to-thickness ratio of a specimen required to achieve a "uniform" orientation. For example, for a ratio of 10 to 1 $\overline{\cos^2 \phi} = 0.93$, and the interpretation of σ_{apparent} as σ_a would result in only 0.07% error when $|\sigma_a - \sigma_t| = 0.01\ \sigma_t$. As the difference $\sigma_a - \sigma_t$ increases, the computed values of $\overline{\cos^2 \phi}$ decrease slightly, as shown in Table 1.

TABLE I

Values of $\cos^2 \phi$ computed from Eq. (2)

L_z/L_x	$\sigma^1 = 0.001$	0.01	0.03	0.1	0.3
1.0	0.340	0.339	0.338	0.333	0.323
0.75	0.505	0.505	0.504	0.501	0.495
0.50	0.655	0.655	0.655	0.653	0.650
0.40	0.721	0.721	0.720	0.720	0.718

If external forces (e.g. magnetic, electric, flow) are present, then the simpler one dimensional analysis[1,2,6] is adequate. Without external forces, however, the orientation of the liquid crystal on the side wall is important, except in thin layers as deduced from Eq. (3).

Appendix

The differential equations, Eq. (1), governing the director orientation is expanded here for a three dimensional problem. We define

$$\mathbf{n} = \sin\phi(\cos\theta\mathbf{e}_x + \sin\theta\mathbf{e}_y) + \cos\phi\mathbf{e}_z,$$

$$\mathbf{n}_\phi = \frac{\partial\mathbf{n}}{\partial\phi} = \cos\phi(\cos\theta\mathbf{e}_x + \sin\theta\mathbf{e}_y) - \sin\phi\mathbf{e}_z,$$

$$\mathbf{n}_\theta = \frac{\partial\mathbf{n}}{\partial\theta} = \sin\phi(-\sin\theta\mathbf{e}_x + \cos\theta\mathbf{e}_y).$$

$$\mathbf{n}_{\phi\theta} = \frac{\partial\mathbf{n}\phi}{\partial\theta} = \cos\phi(-\sin\theta\mathbf{e}_x + \cos\theta\mathbf{e}_y).$$

Then

$$\nabla\mathbf{n} = \nabla\phi\mathbf{n}_\phi + \nabla\theta\mathbf{n}_\theta,$$
$$\nabla\mathbf{n}_\phi = -\nabla\phi\mathbf{n} + \nabla\theta\mathbf{n}_{\phi\theta},$$
$$\nabla\mathbf{n}_\theta = \nabla\phi\mathbf{n}_{\phi\theta} - \nabla\theta(\mathbf{n} - \cos\phi\mathbf{e}_z).$$

The terms in Eq. (1) can then be written in terms of the above. For example,

$$\mathbf{n}x\nabla^2\mathbf{n} = \nabla^2\phi\mathbf{n}x\mathbf{n}_\phi + 2\nabla\phi\cdot\nabla\theta\mathbf{n}x\mathbf{n}_{\phi\theta} + \nabla^2\theta\mathbf{n}x\mathbf{n}_\theta + \nabla\theta\cdot\nabla\theta\cos\phi\mathbf{n}x\mathbf{e}_z.$$

The other terms are developed in a similar fashion. The resulting vector equation is contracted successively with $\mathbf{n}x\mathbf{n}_\phi$ and $\mathbf{n}x\mathbf{n}_\theta$ to obtain the desired coupled partial differential equations in ϕ and θ:

$$\begin{aligned}\gamma_1\frac{\partial\phi}{\partial t} &= k_{22}\{\nabla^2\phi - \sin\phi\cos\phi\nabla\theta\cdot\nabla\theta\}\\ &+ (k_{11} - k_{22})\{(\mathbf{n}_{\phi\theta}\cdot\nabla\theta - \mathbf{n}\cdot\nabla\phi)\mathbf{n}_\phi\cdot\nabla\phi + (\mathbf{n}_{\phi\theta}\cdot\nabla\phi - \mathbf{n}\cdot\nabla\theta\\ &+ \cos\phi\mathbf{e}_3\cdot\nabla\theta)\mathbf{n}_\phi\cdot\nabla\theta + \mathbf{n}_\phi\mathbf{n}_\phi : \nabla\nabla\phi + \mathbf{n}_\phi\mathbf{n}_\phi : \nabla\nabla\theta\}\\ &+ (k_{33} - k_{22})\{(\mathbf{n}_\phi\cdot\nabla\phi + \mathbf{n}_\theta\cdot\nabla\theta)\mathbf{n}\cdot\nabla\phi + \mathbf{n}\cdot\nabla\theta\mathbf{n}_\theta\cdot\nabla\phi\\ &+ \mathbf{n}\mathbf{n} : \nabla\nabla\phi - \sin\phi\cos\phi(\mathbf{n}\cdot\nabla\theta)^2 - \sin^2\phi\mathbf{n}\cdot\nabla\theta\mathbf{n}_\phi\cdot\nabla\theta\}\end{aligned}$$

$$\gamma_1 \sin^2 \phi \frac{\partial \theta}{\partial t} = k_{22}\{\sin^2 \phi \nabla^2 \theta + 2 \sin \phi \cos \phi \nabla \phi \cdot \nabla \theta\}$$

$$+ (k_{11} - k_{22})\{(\mathbf{n}_{\phi\theta} \cdot \nabla \theta - \mathbf{n} \cdot \nabla \phi \mathbf{n}_\theta \cdot \nabla \phi$$

$$+ (\mathbf{n}_{\phi\theta} \cdot \nabla \phi - \mathbf{n} \cdot \nabla \theta + \cos \phi \mathbf{e}_3 \cdot \nabla \theta)\mathbf{n}_\theta \cdot \nabla \theta$$

$$+ \mathbf{n}_\theta \mathbf{n}_\phi : \nabla\nabla \phi + \mathbf{n}_\theta \mathbf{n}_\theta : \nabla\nabla \theta\}$$

$$+ (k_{33} - k_{22})\{\sin^2 \phi[\mathbf{n}_\phi \cdot \nabla \phi \mathbf{n} \cdot \nabla \theta + 2\mathbf{n}_\theta \cdot \nabla \theta \mathbf{n} \cdot \nabla \theta$$

$$+ \mathbf{n} \cdot \nabla \phi \mathbf{n}_\phi \cdot \nabla \theta + \mathbf{n}\mathbf{n} : \nabla\nabla \theta] + 2 \sin \phi \cos \phi \mathbf{n} \cdot \nabla \phi \mathbf{n} \cdot \nabla \theta$$

$$- \mathbf{n} \cdot \nabla \phi \mathbf{n}_\theta \cdot \nabla \phi - \sin^2 \phi \mathbf{n} \cdot \nabla \theta \mathbf{n}_\theta \cdot \nabla \theta\} \tag{4}$$

In these equations, for example,

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$

and

$$\mathbf{n} \cdot \nabla \phi = \sin \phi \left(\cos \theta \frac{\partial \phi}{\partial x} + \sin \theta \frac{\partial \phi}{\partial y} \right) + \cos \phi \frac{\partial \phi}{\partial z}.$$

The three planes $x = 0$, $y = 0$, and $z = 0$ are planes of symmetry, so that

$$\frac{\partial \phi}{\partial x} = \frac{\partial \theta}{\partial x} = 0 \qquad \text{at } x = 0,$$

$$\frac{\partial \phi}{\partial y} = \frac{\partial \theta}{\partial y} = 0 \qquad \text{at } y = 0,$$

$$\frac{\partial \phi}{\partial z} = \frac{\partial \theta}{\partial z} = 0 \qquad \text{at } z = 0,$$

and because $L_x = L_y$,

$$\theta(y, x, z) = \pi/2 - \theta(x, y, z); \quad \theta(x = y) = \pi/4.$$

The surface boundary conditions are described in the text. On the surface $z' = 1$ ($z = L_z/2$) the value of θ is indeterminant, and the value $\pi/4$ is taken as the average of θ on the boundaries at $y' = 1$ and $x' = 1$. At the octant's exterior edges or corners we adopt boundary conditions averaged over adjoining planes or edges, respectively. We note that these edge or corner boundary conditions correspond to singularities in the distortion free energy, since the θ and ϕ gradients are infinite there. However, the affected volume is infinitesimally small so that we assume the free energy integrated over the octant volume is finite. In this sense the boundary conditions are a mathematical idealization.

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