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

A Study of Smectics in a Confined Geometry

Claire Anderson [a] & Frank M. Leslie [a]

[a] Department of Mathematics, University of Strathclyde, Livingstone Tower, 26 Richmond Street, Glasgow, G1 1XH, Scotland

Version of record first published: 24 Sep 2006

To cite this article: Claire Anderson & Frank M. Leslie (1999): A Study of Smectics in a Confined Geometry, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 330:1, 609-616

To link to this article: http://dx.doi.org/10.1080/10587259908025640

Mol. Cryst. Liq. Cryst., 1999, Vol. 330, pp. 609-616
Reprints available directly from the publisher
Photocopying permitted by license only

A Study of Smectics in a Confined Geometry

CLAIRE ANDERSON and FRANK M. LESLIE

Department of Mathematics, University of Strathclyde, Livingstone Tower, 26 Richmond Street, Glasgow G1 1XH, Scotland

This paper discusses a continuum theory for smectic liquid crystals that allows variations in layer spacing and cone angle.

Keywords: smectics; continuum model; layer tilt; layer deformation; strong anchoring

INTRODUCTION

Recently McKay and Leslie[1] discussed a theory for smectics that allows some variation in layer spacing as well as molecular tilt in order to examine configurations beyond the scope of an earlier constrained theory proposed by Leslie et al[2]. With this theory they modelled a smectic C liquid crystal confined in a cell such that its layers are coplanar with the boundary plates, but subject to strong anchoring incompatible with the smectic C tilt. Subsequently Mazzulla and Sambles[3] found good agreement between the theoretical predictions and their experimental observations. Here we consider a smectic A liquid crystal in the bookshelf geometry, but subject to a strongly anchored pretilt at the plates, a configuration discussed experimentally by Elston[4], and one that offers further possibilities for comparison between theory and experiment.

DESCRIPTION OF SMECTIC CONFIGURATION

We consider an infinite planar sample of smectic A liquid crystal bounded by two plates a distance of $2d$ apart (see Figure 1). The molecules are strongly anchored in the xz-plane at the boundaries, causing the smectic layers to bend, and inducing some tilt of alignment with respect to the layer normal.

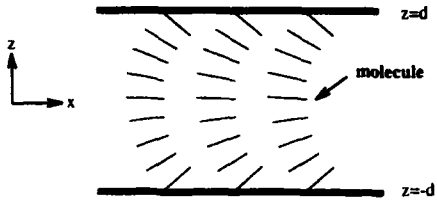

FIGURE 1 Strong anchoring at plates forcing SmC type behaviour near the boundaries.

Layer Tilt

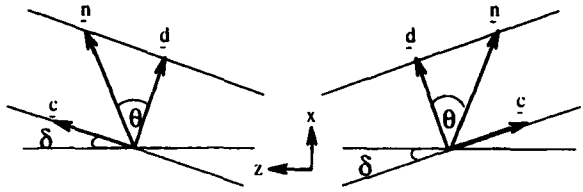

FIGURE 2(a) Description of molecule directors.

It is reasonable to assume that there is no domain structure parallel to the plates and thus all angles vary only with respect to the z coordinate. The angle δ describes the layer tilt, and in this case is chosen to lie between $-\pi/2$ and $\pi/2$. More precisely, $\delta(z) > 0$ in the upper half, and $\delta(z) < 0$ in the lower half of the cell. Note that for symmetry and continuity in the centre of the sample, it is required that $\delta(0)$ vanishes (see Figure 1).

The vector $\underline{n}$ represents the mean direction of the liquid crystal molecules, and to simplify the model, it is sensible to assume that $\underline{n}$ is of unit length and rescale all other lengths accordingly. The "layer thickness" vector $\underline{d}$ is orthogonal to the smectic layer and has magnitude equal to the rescaled layer spacing. Further, $\underline{c}$ is simply the projection of $\underline{n}$ onto the smectic layer, thus $\underline{c}$ and $\underline{d}$ are orthogonal.

Our in-plane description of the liquid crystal molecules is complete when the SmC cone angle $\theta(z)$ is introduced. This is the angle between the director and the layer normal, and is assumed to be an acute angle. If $\theta(z)$ is zero, the molecules are clearly in the SmA phase, while $\theta(z)$ non-zero, indicates a SmC type configuration.

Twist Angle

To conclude the three dimensional description of the directors, it is necessary to introduce a twist angle $\phi(z)$ which allows the molecules to come out of

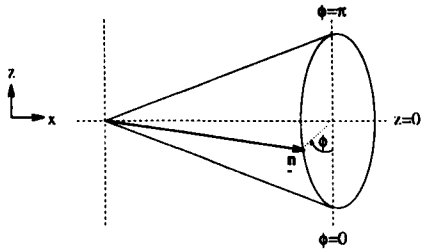

FIGURE 2(b) Description of molecule directors.

the plane as shown in Figure 2(b). Here we assume that $0 \leq \phi(z) \leq \pi$, but equally any range $k\pi \leq \phi(z) \leq (k+1)\pi$, $k \in Z$ may be used.
The directors $\underline{d}$, $\underline{c}$ and $\underline{n}$ may therefore be described as follows:
$\underline{d} = \cos\theta(\cos\delta,\ 0,\ -\sin\delta)$
$\underline{c} = -\sin\theta(\sin\delta\cos\phi,\ \sin\phi,\ \cos\delta\cos\phi)$
$\underline{n} = (\cos\theta\cos\delta - \sin\theta\sin\delta\cos\phi,\ -\sin\theta\sin\phi,\ -\cos\theta\sin\delta - \cos\delta\cos\phi\sin\theta)$.
In the analysis, the density wave vector $\underline{a}$ is used in preference to $\underline{d}$. This is simply a vector in the direction of $\underline{d}$ with magnitude $2\pi/|\underline{d}|$

$$\text{i.e.} \quad \underline{a} = \frac{2\pi}{\cos\theta}(\cos\delta,\ 0,\ -\sin\delta).$$

CONSTRAINTS

In the absence of defects (no dislocation of layers), the density wave vector $\underline{a}$ is subject to the constraint that curl $\underline{a}$ is zero, which in our case imposes the condition

$$\cos\delta = k\cos\theta \tag{1}$$

for $k > 0$, and $\underline{a}$ may be rewritten as $\underline{a} = 2\pi k(1,\ 0,\ -\tan\delta)$.
A further restriction imposed by our model is that n_3, the z-component of the director, is equal to zero at the centre in order to ensure symmetry and continuity of $\underline{n}$ throughout the sample.

$$\text{i.e.} \quad \cos\phi_0 = -\frac{\tan\delta_0}{\tan\theta_0}, \quad \theta_0 \neq 0, \tag{2}$$

where the zero subscript denotes the value at $z = 0$.
Given the value of k, the above two conditions do in fact give a great deal of information about the nature of the solutions. From (1) and (2) we deduce that $k \geq 1$, but physically k is required to be not much greater than 1.
We consider the two cases $k = 1$ and $k > 1$ as follows:
$\underline{k = 1}$: In this case equation (1) implies that δ is equal to $\pm\theta$, and one can have in-plane symmetric solutions in which

$$\delta = \theta, \quad \phi = \pi, \quad z > 0; \quad \delta = -\theta, \quad \phi = 0, \quad z < 0$$
$$\text{or} \quad \delta = \theta, \quad \phi = 0, \quad z > 0; \quad \delta = -\theta, \quad \phi = \pi, \quad z < 0$$

with both δ and θ zero at $z = 0$.

$\underline{k > 1}$: In this case θ does not vanish at $z = 0$, although δ does, and therefore for a symmetric solution

$$\cos\phi_0 = 0 \quad \text{or} \quad \phi_0 = \frac{\pi}{2}$$

with the alignment clearly coming out of the xz-plane.

GOVERNING EQUATIONS

In the bulk of the sample, balance of angular momentum requires that

$$\left(\frac{\partial W}{\partial c_{i,j}}\right)_{,j} - \frac{\partial W}{\partial c_i} + \mu a_i + \gamma c_i = 0 \tag{3}$$

$$\left(\frac{\partial W}{\partial a_{i,j}}\right)_{,j} - \frac{\partial W}{\partial a_i} + \mu c_i - \frac{4\pi^2}{(\underline{a}.\underline{a})^2}\gamma a_i + \epsilon_{ijk}\beta_{k,j} = 0 \tag{4}$$

where μ, γ and $\underline{\beta}$ are Lagrange multipliers, and Cartesian tensor notation is employed throughout.

W is the bulk energy of the sample, but for simplicity we do not consider the complete elastic energy which requires rather more elastic constants, and instead use the following form:

$$2W = K^a (a_{i,i})^2 + K (c_i c_i)^2 + K^c (c_{i,j} c_{i,j}) . \tag{5}$$

This particular form has been chosen in order to take into account the three most important features of the model; the terms K^a, K and K^c respectively being measures of layer elasticity, departures from SmA behaviour, and distortions of the director around the layer normal. In this case, the elastic constants are such that $K^c \ll K^a \ll K$.

SOLUTIONS

For our particular model, equations (3) and (4) yield

$$K^c c_{i,pp} - 2K c_p c_p c_i + \mu a_i + \gamma c_i = 0 \tag{6}$$

$$K^a a_{p,pi} + \mu c_i - \frac{4\pi^2}{(\underline{a}.\underline{a})^2}\gamma a_i + \epsilon_{ijk}\beta_{k,j} = 0. \tag{7}$$

Each of the previous two vector equations may be analysed to extract expressions for the Lagrange multipliers as follows:

μ and γ are obtained from equation (6).

$$\underline{a} \cdot (6) \Rightarrow \mu = \frac{K^c}{2\pi}\cos\theta\,(2\theta'\delta'\cos\theta\cos\phi + \delta''\sin\theta\cos\phi - 2\delta'\phi'\sin\theta\sin\phi)$$

$$\underline{c} \cdot (6) \Rightarrow \gamma = 2K\sin^2\theta - K^c\left(\theta''\cot\theta - \theta'^2 - \delta'^2\cos^2\phi - \phi'^2\right)$$

The above two expressions now allow $\underline{\beta}$ to be found from equation (7). If the scalar product of equation (6) and $(\underline{a} \times \underline{c})$ is taken, this yields the following differential equation:

$$\phi'' \sin\theta + 2\theta'\phi' \cos\theta + \delta'^2 \sin\theta \sin\phi \cos\phi = 0. \tag{8}$$

We return to the above equation at a later stage, and regard it as a second order differential equation for $\phi(z)$. For the moment, however, we turn our attention to finding an equation for $\delta(z)$. At this stage, for simplicity it is convenient to rescale $z \to zd$. Supposing that $K^c \ll K^a$, equation (7) yields to first approximation

$$\delta'' \sec^2\delta + 2\delta'^2 \sec^2\delta \tan\delta = \frac{Kd^2}{2\pi^2 k^4 K^a}\left(1 - \frac{\cos^2\delta}{k^2}\right)\cos^3\delta \sin\delta$$

Integrating the above expression gives

$$\delta'^2 \sec^4\delta = \frac{\alpha^2}{k^2}\left(1 - \frac{\cos^2\delta}{k^2}\right)^2 + C, \quad \text{where} \quad \alpha^2 := \frac{Kd^2}{4\pi^2 K^a}.$$

and C is simply a constant of integration. Since this particular model requires that the layer tilt δ be positive in the upper half and zero in the centre, this implies that $\delta'(0) > 0$. Let $\delta'(0) = \alpha\lambda/k > 0$, to give the following first order differential equation for $\delta(z)$:

$$\frac{d\delta}{dz} = \frac{\alpha}{k}\cos^2\delta \sqrt{\left(1 - \frac{\cos^2\delta}{k^2}\right)^2 + \lambda^2 - \left(1 - \frac{1}{k^2}\right)^2}. \tag{9}$$

Thus, if the values of k, α, d and the fixed boundary condition $\delta(d)$ are known, then one may calculate the layer tilt at each point in the cell.

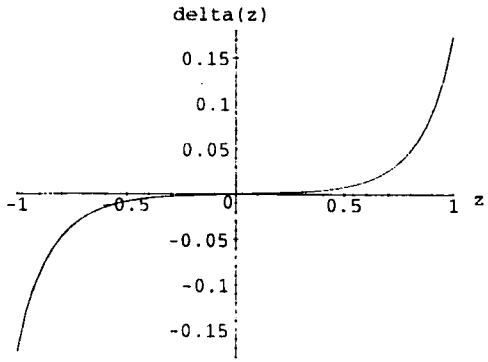

FIGURE 3 Graph of $\delta(z)$ when we have the fixed parameters $k = 1.01, d = 1, \alpha = 30, \delta(d) = 10°$.

Note the apparently simple form of the equation when we have the in-plane solution with k equal to unity:

$$\frac{d\delta}{dz} = \alpha \cos^2 \delta \sqrt{\sin^4 \delta + \lambda^2}.$$

Frustratingly enough, we have been unable to solve even this form of the equation analytically, and in all cases have had to resort to numerical techniques to obtain solutions. Figure 3 shows one such numerical solution.
The alignment of the molecules in the cell is very dependent upon how they are fixed at the boundaries. We now look at the different configurations which arise if we anchor the molecules either parallel or at an angle to the plates.

Molecules Anchored Parallel to the Plates

If the molecules are anchored parallel to the plates, they will remain so throughout the sample, and we are forced to have $k = 1$. There are 2 cases depending on whether $\delta(d)$ is zero or non-zero:
(a) Figure 4(a) shows the configuration when $\delta(d) = \theta(d) = 0$, and hence $\delta(z)$ and $\theta(z)$ are zero throughout the sample.
(b) Figure 4(b) shows the configuration when $\delta(d) \neq 0$ and thus

$$\delta = \theta, \quad \phi = \pi, \quad z > 0; \quad \delta = -\theta, \quad \phi = 0, \quad z < 0.$$

In this case, $\delta(z)$ and hence $\theta(z)$, may be found via equations (1) and (9). Clearly the solution (a) has the lower energy.

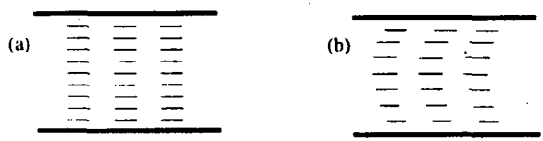

FIGURE 4 Possible geometric configurations when molecules are anchored parallel to the plates.

Molecules Anchored at an Angle to the Plates

If we anchor the molecules at an angle to the plates at the boundaries, then again there are 2 cases to consider:
$k = 1$: Here we choose the second option discussed earlier for solutions with alignment in the xz-plane

i.e. $\delta = \theta, \quad \phi = 0, \quad z > 0; \quad \delta = -\theta, \quad \phi = \pi, \quad z < 0.$

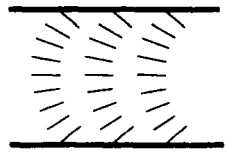

FIGURE 5 Possible geometric configuration when $k = 1$.

$\delta(z)$ is governed by equation (9) with a suitable fixed boundary condition (see Figure 5). Since the cone angle $\theta(z)$ is necessarily zero at $z = 0$, it is unimportant as to whether ϕ_0 is equal to 0 or π.

$k > 1$: In this case, the molecules are forced out of the plane, and $\phi(0) = \pi/2$. In order to see how $\phi(z)$ varies, equation (8) is written in terms of δ and ϕ alone as follows:

$$\phi''\sqrt{1-\frac{\cos^2\delta}{k^2}} + 2\phi'\frac{\delta'\cos\delta\sin\delta}{k\sqrt{k^2-\cos^2\delta}} + \delta'^2\sqrt{1-\frac{\cos^2\delta}{k^2}}\sin\phi\cos\phi = 0$$

and since $k > 1$, one may divide through by $\sqrt{1-\frac{\cos^2\delta}{k^2}}$ to give

$$\phi'' + \phi'\frac{\delta'\sin 2\delta}{k^2-\cos^2\delta} + \frac{1}{2}\delta'^2\sin 2\phi = 0. \tag{10}$$

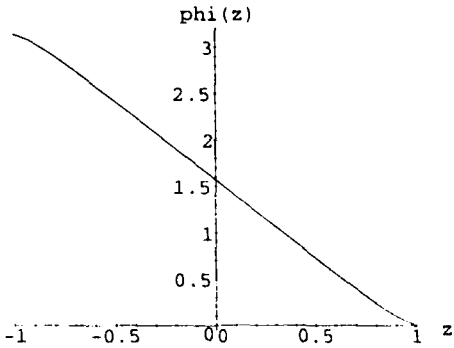

FIGURE 6 Graph of $\phi(z)$ when we have the fixed parameters $k = 1.01, d = 1, a = 30, \delta(d) = 10^o$.

A numerical solution for $\delta(z)$ has already been computed in FORTRAN and thus we may regard equation (10) as a differential equation for $\phi(z)$, which may in turn be solved numerically. Figure 6 shows one such numerical solution.

Continuity of Stress and Couple Stress

We must ensure that the solutions which we have obtained are continuous in both stress and couple stress across the centre of the sample. The required continuity conditions are trivially satisfied if $k \neq 1$. If however $k = 1$, even though the director is continuous, there is a discontinuity in $\phi(z)$ at $z = 0$. Consequently, $\phi'(0)$ does not exist, but it may be shown that relevant components of stress and couple stress do in fact vary continuously as required. One may therefore conclude that stress and couple stress are continuous, and our solutions do indeed describe equilibrium configurations.

Energy Considerations

After having found several different mathematically correct equilibrium solutions, it is necessary to consider those which are physically relevant. It is thus essential to identify those solutions which are more energetically favourable. The energy of the system is computed via the equation

$$\text{Energy} = \int_d^d W dz$$

where W is given by equation (5). For our particular model, and again assuming that $K^c \ll K^a$, this expression may be reduced to an integral of the form

$$\text{Energy} = Kd \int_0^1 \left\{ 2\left(1 - \frac{\cos^2\delta}{k^2}\right)^2 + \lambda^2 - \left(1 - \frac{1}{k^2}\right)^2 \right\} dz.$$

Independent of the choice of boundary conditions and elastic constants, it can be shown that the energy is always a minimum when $k = 1$. In conclusion therefore, we have found the in-plane solution to be the more energetically favourable of the solutions with pretilt discussed here, although there may be others not discussed with lower energy. This is in agreement with experimental results obtained by Elston[4], which showed that configurations of this kind never came out of the plane.

Acknowledgements

This work was carried out with financial support from the U.K. Engineering and Physical Sciences Research Council and DERA, Malvern.

References

[1] G. McKay and F.M. Leslie, *Euro. Jnl. Appl. Maths.*, **8** 273 (1997).
[2] F.M. Leslie, I.W. Stewart and M. Nakagawa, *Mol. Cryst. Liq. Cryst.*, **198** 443 (1991).
[3] A. Mazzulla and J.R. Sambles, *Liq. Cryst.*, **22** 727 (1997).
[4] S.J. Elston, *Liq. Cryst.*, **16** 151 (1994).