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A continuum theory for smectic liquid crystals allowing layer dilation and compression

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We present a continuum theory for smectic liquid crystals which allows variable molecular tilt and layer spacing by relating the two. This compressible theory is employed to predict the effect of 'homeotropic' type ordering at the plates on a planar Sm C sample. Such a boundary condition induces dilation of individual Sm C layers near the bounding plates.

1 Introduction

Most early theoretical studies of Sm C liquid crystals exclude variations in the interlayer spacing or changes in molecular tilt with respect to the smectic layer normal (e.g. Carlsson *et al*. [1], Leslie & Gill [2], Stewart *et al*. [3]). In particular Leslie *et al*. [4] present a general nonlinear continuum theory for Sm C liquid crystals based on this constant thickness assumption. This theory has proved useful for mathematical analyses of both static and dynamic problems in a number of different geometries; see the other contributions to this volume. In this paper our aim is to adapt this general theory and its equilibrium equations, applying it to a model for planar Sm C layers where layer spacing (and hence molecular tilt) can vary.

Recently Nakagawa [5, 6] and Mukai & Nakagawa [7] have considered compressible (variable thickness) Sm C liquid crystals in order to describe the appearance of one and two dimensional chevron structures in ferroelectric liquid crystals. Indeed, Nakagawa [8] has extensively studied the elastic properties of such liquid crystals and presented a general free energy to describe their behaviour. Similarly, De Meyere *et al*. [9] also allow thickness variations in their study of chevron profiles in ferroelectrics and the influence of applied voltages. Mechanical instabilities or phase changes between Sm A and Sm C liquid crystals can also be explained via compressible arguments. Ribotta & Durand [10] discuss such instabilities of Sm A liquid crystals under dilative or compressive stresses. Two forms of instability are possible: undulation of the layers; or molecular tilt inside the layers. Another compressible effect has recently been reported by Elston [11] for a Sm A sample in a bookshelf geometry with high surface pretilt. In that experiment, the surface tilt induces a Sm A to Sm C phase change as the orientation of the molecule varies and the layers bend.

This paper presents a theoretical analysis of a compressible Sm C sample where each smectic layer is parallel to the boundary plates, with an imposed 'homeotropic' type ordering at the plates via a strong anchoring condition on the molecules. Such a boundary condition induces compression or dilation of individual Sm C layers as the molecule tilt varies throughout the sample. We derive an expression for molecular tilt throughout the

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layer by utilizing a general continuum theory similar to that of Leslie *et al*. [4], taking into account the different constraints imposed upon the sample in the compressible model.

2 Description

We represent a liquid crystal molecule via a unit vector $\boldsymbol{n}$. To describe the layered structure in a Sm C liquid crystal we also employ a 'layer thickness' vector $\boldsymbol{d}$ which is normal to the smectic layer and has magnitude equal to the (rescaled) layer spacing. We further define a vector $\boldsymbol{c}$ which is the projection of $\boldsymbol{n}$ onto the smectic layer (see Figure 1). From Figure 1 we see that in fact

$$\boldsymbol{n} = \boldsymbol{d} + \boldsymbol{c}. \tag{1}$$

The density wave vector, $\boldsymbol{a}$, is now a vector with magnitude $2\pi/|\boldsymbol{d}|$ in the direction of $\boldsymbol{d}$, i.e.

$$\boldsymbol{a} = \frac{2\pi}{\boldsymbol{d}\cdot\boldsymbol{d}}\boldsymbol{d}. \tag{2}$$

As in previous analyses of Sm C liquid crystals where the smectic layers were assumed to be of constant thickness (e.g. [3, 4]), in the absence of defects the density wave vector is subject to the constraint $\nabla \times \boldsymbol{a} = 0$ (Oseen [12]).

Moreover, from the definitions of $\boldsymbol{n}$, $\boldsymbol{a}$ and $\boldsymbol{c}$, our vectors are also constrained via

$$\boldsymbol{a}\cdot\boldsymbol{c} = 0, \quad \boldsymbol{n}\cdot\boldsymbol{n} = \boldsymbol{d}\cdot\boldsymbol{d} + \boldsymbol{c}\cdot\boldsymbol{c} = \frac{4\pi^2}{\boldsymbol{a}\cdot\boldsymbol{a}} + \boldsymbol{c}\cdot\boldsymbol{c} = 1. \tag{3}$$

Assuming the sample temperature is *fixed*, the equilibrium equations (essentially, the equations for balance of angular momentum [4]) in the bulk of the sample are

$$\Pi_i^a + \mu\, c_i - \frac{4\pi^2}{(\boldsymbol{a}\cdot\boldsymbol{a})^2}\gamma\, a_i + \epsilon_{ijk}\beta_{k,j} = 0, \tag{4}$$

$$\Pi_i^c + \mu\, a_i + \gamma\, c_i = 0, \tag{5}$$

where

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

μ, γ and $\boldsymbol{\beta}$ are Lagrange multipliers which appear as a result of constraints (3); W is the bulk elastic energy of the sample; and we have employed standard indicial notation. Equations (4), (5) differ from those for an incompressible (constant layer thickness) smectic because of the different definitions and constraints imposed upon $\boldsymbol{a}$ and $\boldsymbol{c}$; see the article by Atkin and Stewart in this volume, where the notation differs from ours. It now remains to choose an appropriate form for the bulk energy

$$W = W(\boldsymbol{a}, \boldsymbol{c}, \nabla\boldsymbol{a}, \nabla\boldsymbol{c}).$$

For incompressible smectics it has been shown that nine elastic constants are required to write down the complete elastic energy (assuming an energy quadratic in the gradients of

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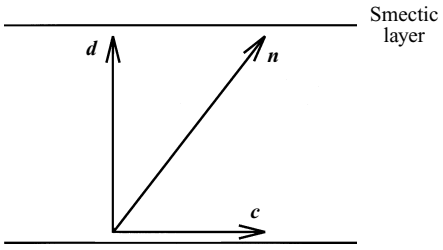


FIGURE 1. Description of molecule directors.

$\boldsymbol{a}$ and $\boldsymbol{c}$). However, for compressible smectic layers the number of constants required is far greater. If we were to employ a complete form of this energy, then our analysis would become complicated, and any meaningful results would be very difficult to obtain.

Instead, we adopt a simple energy which contains a dilation term and products of $\nabla\cdot\boldsymbol{a}$, $\nabla\boldsymbol{a}$, $\nabla\cdot\boldsymbol{c}$ and $\nabla\boldsymbol{c}$ only. This is similar to [8], which formulates a general energy before adopting a simplified form for the analysis and results. Our choice for energy W is

$$2W = K(c_i\,c_i - c_i^o\,c_i^o)^2 + A(a_{i,i})^2 + C\,c_{i,j}\,c_{i,j} - 2B\,a_{i,i}\,c_{j,j}, \tag{6}$$

where K, A, B and C are all elastic constants (non-negative except for B). $\boldsymbol{c}^o$ is the expected $\boldsymbol{c}$ director for our smectic sample when there are *no boundary effects*.

3 Model

To model the effect of a homeotropic type ordering on the plates we consider an infinite planar layer of Sm C liquid crystal bounded by the planes $x = 0$ and $x = h$. Each Sm C layer within the sample is parallel to these planes (see Figure 2).

Defining tilt angle θ to be the angle between the layer normal and the molecule director, we can now represent the vectors $\boldsymbol{d}$, $\boldsymbol{a}$, $\boldsymbol{c}$ and $\boldsymbol{n}$ via

$$\begin{aligned} \boldsymbol{d} &= \cos\theta\,(1,0,0), \quad \boldsymbol{a} = \frac{2\pi}{\cos\theta}(1,0,0), \\ \boldsymbol{c} &= \sin\theta\,(0,1,0), \quad \boldsymbol{n} = (\cos\theta, \sin\theta, 0). \end{aligned} \tag{7}$$

It is reasonable to assume that within each smectic layer molecules are parallel. Hence θ is allowed to vary only with the vertical coordinate x.

Following the discussion in the previous section, we define

$$\boldsymbol{c}^o = (0, \sin\theta_o, 0), \tag{8}$$

where θ_o is the equilibrium value for cone angle θ. θ_o is the constant value of θ we would expect when there are no external influences. The dilation term $K(\boldsymbol{c}\cdot\boldsymbol{c} - \boldsymbol{c}^o\cdot\boldsymbol{c}^o)^2$ in W is therefore a measure of the energy lost as θ deviates from θ_o.

Finally, we introduce homeotropic type ordering on our boundary plates by forcing

$$\theta = \theta_w \quad \text{on} \quad x = 0 \quad \text{and} \quad x = h. \tag{9}$$

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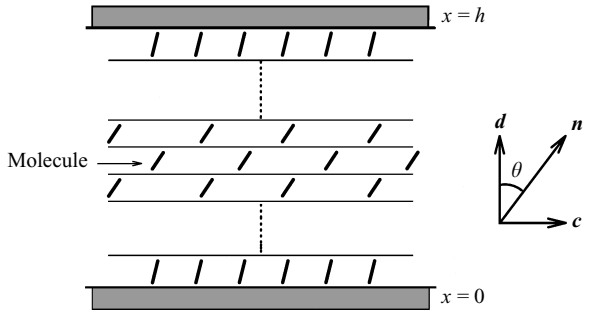


FIGURE 2. Homeotropic type ordering on the plates for a planar Sm C layer.

By introducing the angle $\theta_w \not\equiv \theta_o$, the sample can no longer exhibit a constant equilibrium tilt throughout the layer. Instead, the layers near the plates are more dilated because the molecules line up with the sample normal. We assume this effect takes place at a fixed temperature, and that any changes in molecule tilt are mechanical.

Although we have fixed the tilt at the boundaries, an alternative approach allows each plate to exhibit a finite surface energy of the form

$$w_s = -\sigma(\boldsymbol{v}\cdot\boldsymbol{n})^2,$$

where $\boldsymbol{v} = (1,0,0)$ is normal to the bounding surfaces and σ (>0) is an elastic constant. (This choice of w_s is minimized when $\boldsymbol{n}$ is parallel to $\boldsymbol{v}$, i.e. Sm A ordering.)

Balance of couples at the boundary allows us to find boundary conditions for $\mathrm{d}\theta/\mathrm{d}x$, which we solve in conjunction with the ordinary differential equations for the bulk. However, this approach adds another elastic constant to our analysis, making any numerics more complicated. In this analysis, we concentrate on the simpler approach of *fixing* $\theta = \theta_w$ on the plates.

4 Solution

Substituting (6), (7) and (8) into (5), we immediately see that

$$\left.\begin{aligned} \mu &= B\cos\theta\,(\sec\theta)'', \\ \gamma &= 2K(\sin^2\theta - \sin^2\theta_o) - C\frac{(\sin\theta)''}{\sin\theta}, \end{aligned}\right\} \tag{10}$$

where $'$ represents $\mathrm{d}/\mathrm{d}x$. The assumption that tilt varies only with x in turn suggests that multiplier $\boldsymbol{\beta}$ should only depend on x. Substituting into (4), we have the following:

$$\left.\begin{aligned} &\beta_1 = 0, \quad \beta_2 = 0, \\ &\beta_3 = B\sin\theta\cos\theta\,(\sec\theta)' - B\,R(x), \end{aligned}\right\} \tag{11}$$

where

$$R(x) = \int_{h/2}^{x} \sin\theta\,(1-\tan^2\theta)(\theta')^2\,ds$$

is chosen to ensure β_2 is anti-symmetric about the centre of the sample.

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To simplify our analysis we may rescale our vertical coordinate via $x \to hx$. Equation (4) now finally reduces to

$$\left(\frac{\sin\theta}{\cos^2\theta}+F^2\frac{\cos^4\theta}{\sin\theta}\right)\theta''+\left(\frac{1+\sin^2\theta}{\cos^3\theta}-F^2\cos^3\theta\right)(\theta')^2-D^2\cos^3\theta(\sin^2\theta-\sin^2\theta_o)=0, \quad (12)$$

$$\theta=\theta_w \quad \text{on} \quad x=0 \quad \text{and} \quad x=1,$$

where
$$D^2=\frac{Kh^2}{2\pi^2 A}, \quad F^2=\frac{C}{4\pi^2 A}$$

are ratios of the elastic constants, and now $\theta=\theta(x)$, $0 \leqslant x \leqslant 1$.

In general, we cannot solve this system analytically, and we resort to numerical integration. An analytical solution is possible when $F^2=0$. In this case we may integrate (12) to give

$$(\theta')^2=\frac{D^2\cos^4\theta}{2\sin^2\theta}(\cos^2\theta-\cos^2\theta_m)(\cos^2\theta+\cos^2\theta_m-2\cos^2\theta_o), \quad (13)$$

where $\theta_m=\theta(1/2)$. Integrating once more, we can express θ_m in the closed form

$$\int_{\theta_w}^{\theta_m}\frac{\sin\theta}{\cos^2\theta\, M(\theta)}\mathrm{d}\theta=\frac{D}{2\sqrt{2}}, \quad (14)$$

with
$$M(\theta)=[(\cos^2\theta-\cos^2\theta_m)(\cos^2\theta+\cos^2\theta_m-2\cos^2\theta_o)]^{1/2}.$$

Integrated equations (13) and (14) assume $\theta'=0$ in the middle of the sample. This is a natural assumption to make as we require $\theta=\theta_w$ on both boundary plates; thus solutions may be sought which are symmetric around the middle of the layer. However, in future analyses we may allow θ to have distinct values on each plate, and this symmetry assumption would no longer be valid. The integral in equation (14) can be rewritten as the sum of elliptic integrals of first and second kind. A boundary layer analysis is not justified in the present examination of this simplified application.

The constant F^2 is proportional to the elastic constant for the ***c***-director deformation energy. For the Sm C sample we consider we expect $\theta \simeq \theta_o$ in a large proportion of the layer. Since K is the elastic constant associated with compression of smectic layers and the deviation of θ from θ_o, we expect the influence of our dilation energy in W to be much greater than that of the ***c***-director contribution, i.e. we expect $Kh^2 \gg C$. Thus the assumption that $F^2=0$, allowing us to calculate an analytical solution, is a physically realistic one. Indeed, our numerical results verify that our solutions for $F^2=0$ and $F^2 \neq 0$ are qualitatively similar. The analytical solution provides a useful guide to the behaviour as we vary D^2, θ_o and θ_w.

5 Discussion

Figures 3–5 show numerically calculated solutions $\theta(x)$ for system (12). In particular, they demonstrate the effect of variable elastic constant D^2 and angles θ_o, θ_w on molecular tilt.

Figures 3 and 4 illustrate the influence of the compression energy in our analysis. As D^2 decreases (i.e. elastic constant K decreases), any deviation of tilt θ from the strainfree value θ_o becomes energetically more favourable and the sample 'relaxes'. For larger K (and hence

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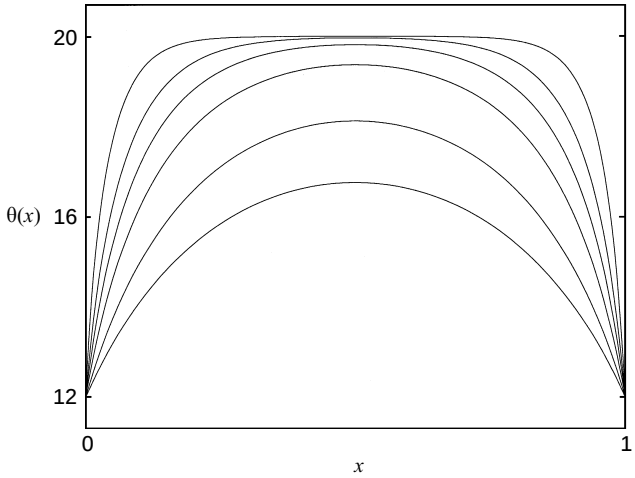


FIGURE 3. Variation of tilt angle θ with D^2 ($\theta_o = 20°$; $F^2 = 0$; $\theta_w = 12°$; $D^2 = 5$ (bottom graph), 10, 25, 50, 100 and 300 (top graph)).

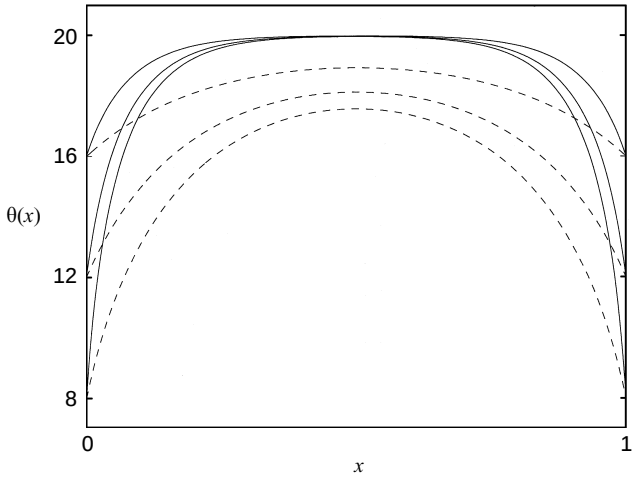


FIGURE 4. Effect of variable θ_w on molecular tilt in the sample ($\theta_o = 20°$; $F^2 = 0$; $\theta_w = 8°$, 12° and 16°; (– – –): $D^2 = 10$; (——): $D^2 = 100$).

larger D^2), $\theta \simeq \theta_o$ in more of the layer as expected, while $\theta_m = \theta(1/2)$ is also greater. Figure 4 also shows that for large D^2, $\theta_m \simeq \theta_o$ even when θ_w is varied.

For a constant boundary tilt θ_w the data in Figure 5 indicates that as θ_o increases, our solutions vary more rapidly near the boundaries. Despite this, there is still very little variation in angle throughout the bulk of the layer. Finally, following the discussion in the previous section we have omitted any results which allow $F^2 \neq 0$.

6 Conclusions

By developing a continuum theory for Sm C liquid crystals where the interlayer spacing is allowed to vary we have attempted to model a planar Sm C sample subject to homeotropic (Sm A type) ordering at the bounding plates. This 'compressible' continuum theory yields

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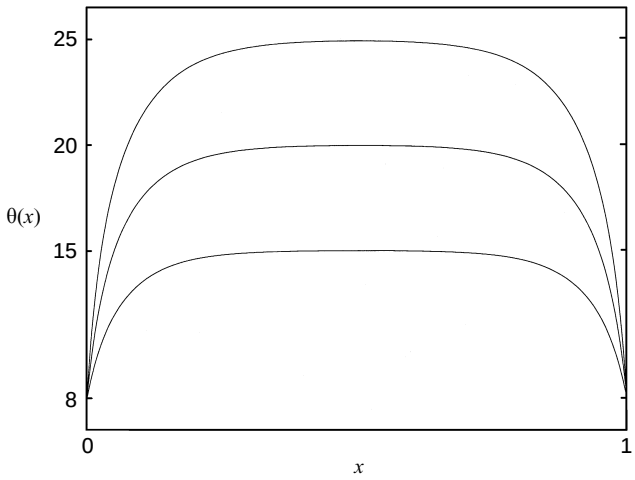


FIGURE 5. Effect of variable equilibrium angle θ_o ($D^2 = 100$; $\theta_w = 8°$; $F^2 = 0$; $\theta_o = 15°$, 20° and 25°).

an expression for the molecular tilt throughout the sample thickness, and predicts the influence of different free energies on our numerical solutions. A similar analysis may now be applied to other smectic geometries, allowing us to model different experimental set-ups and thus obtain predictions for certain material constants.

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