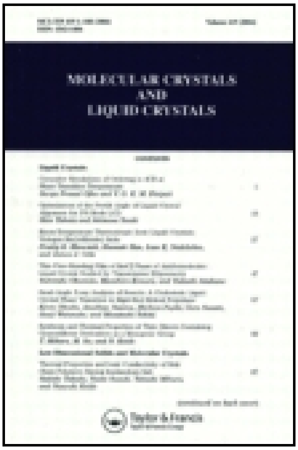

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Finite Planar Domains of Smectic a Liquid Crystals Subjected to Uniform Pressure and Magnetic Fields

Iain W. Stewart [a] & Graeme J. Barclay [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

Mol. Cryst. Liq. Cryst., 1999, Vol. 328, pp. 505-512
Reprints available directly from the publisher
Photocopying permitted by license only

Finite Planar Domains of Smectic a Liquid Crystals Subjected to Uniform Pressure and Magnetic Fields

IAIN W. STEWART and GRAEME J. BARCLAY

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

Theoretical results are presented for finite samples of smectic *A* liquid crystals subjected to both a uniform pressure and a magnetic field applied perpendicular to the smectic layers. A uniform pressure with no field present is also considered. Criteria for suitable boundary conditions are given for planar sample geometries. 'Grid-like' smectic layer undulations are shown to arise as solutions to the governing equilibrium equation.

Keywords: smectic *A*; layer undulations; Helfrich-Hurault instability

INTRODUCTION

We report upon recent theoretical work by the authors[1] for the Helfrich-Hurault transition in samples of smectic *A* liquid crystals in finite rectangular and circular domains subjected to both a uniform pressure and a magnetic field. The incorporation of a pressure term and consideration of finite boundaries therefore extends the results of Helfrich[2] and Hurault[3] for infinite samples of cholesterics which experience undulations above a critical magnetic field strength: details can be found in the books by De Gennes and Prost[4] and Chandrasekhar[5]. Smectic *A* liquid crystals are layered anisotropic fluids. Each layer consists of long molecules whose average molecular alignment is perpendicular to the layers. The average alignment is denoted by the unit vector **n**, called the director. Typical sample alignments are as indicated in Fig.1 where we consider either a smectic *A* in a homeotropic alignment between two plates at a distance *d* apart in the

z-direction and of finite dimensions a and b in the x- and y-directions, or a cylindrical alignment of depth d and radius R, as shown in the Figure. A

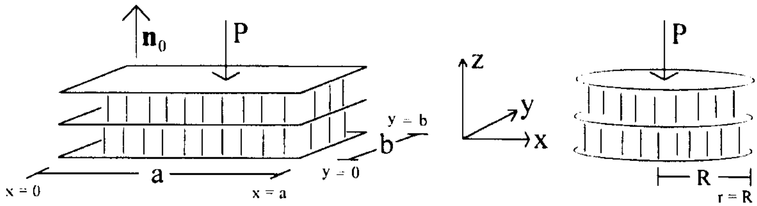

FIGURE 1 Planar samples of smectic A. The average molecular alignment is parallel to the z-axis and the similarly aligned molecules inherent in the smectic A phase form equidistant layers as shown. A uniform constant pressure P is applied across the sample in the negative z-direction. A magnetic field $\mathbf{H}$ may also be present in the z-direction.

small uniform constant pressure P is applied in the negative z-direction as shown and a magnetic field $\mathbf{H}$ may also be present in the z-direction. A field in the x-direction has been discussed elsewhere[6] using a similar approach to that presented here: a one-dimensional rather than a two-dimensional pattern occurs: this agrees with recent work by Fukuda and Onuki[7].

The displacement of the layers is represented in the usual notation by $u(x, y, z)$. The corresponding smectic A bulk elastic energy is[4,p.343]

$$w_A = \frac{\overline{B}}{2}u_z^2 + \frac{K_1}{2}\left[(u_{xx} + u_{yy})^2 + 4(u_{xy}^2 - u_{xx}u_{yy})\right], \tag{1}$$

where $\overline{B}$ is the smectic layer compression constant and K_1 is the usual elastic splay constant. Throughout, suffices denote partial differentiation with respect to the variables indicated. For convenience, the parameter λ is introduced as $\lambda = \sqrt{K_1/\overline{B}}$, which is a characteristic length of the material, of the order of the smectic layer thickness. Following De Gennes and Prost[4], for small displacements to the initial alignment $\mathbf{n}_0$ the director $\mathbf{n}$ will be given by $\mathbf{n} \approx (-u_x, -u_y, 1)$ with $|u_x|, |u_y| \ll 1$. The relevant magnetic energy when $\mathbf{H}$ is applied parallel to the z-axis is[4,p.344],

$$w_{Mz} = \frac{1}{2}\chi_a H^2(u_x^2 + u_y^2). \tag{2}$$

where the constant contribution term has been omitted and $H = |\mathbf{H}|$. Notice that there is no minus sign in (2). It is supposed that the diamagnetic anisotropy χ_a is negative, in which case the director will be repelled by such a field and the layers will compress.

The total energy integral over the volume Ω is

$$W = \int_\Omega (w_A + w_{Mz})d\Omega. \tag{3}$$

We assume that the layer displacements are of small amplitude and that we can make an approximation for u of the form

$$u = u_0 \sin(\frac{\pi}{d}z)\, v(x, y) \tag{4}$$

with u_0 a small constant, allowing u to be zero on the boundaries $z = 0, d$. Inserting (4) into (3) gives

$$W = \frac{1}{2} d u_0^2 \int_S \left[\frac{\overline{B}}{2}\left(\frac{\pi}{d}\right)^2 v^2 + \frac{K_1}{2}(\Delta v)^2 + 2K_1(v_{xy}^2 - v_{xx}v_{yy}) + \frac{1}{2}\chi_a H^2(v_x^2 + v_y^2)\right] dS \tag{5}$$

where S is the corresponding region in the xy-plane with boundary Γ (for example, in Fig. 1, Γ is either a rectangle or circle), and Δ is the usual two dimensional Laplace operator.

We now briefly summarise the method proposed by Stewart[6] for incorporating a uniform pressure into the model. The work done by the constant pressure, which is the constant force P per unit area in the xy-plane on a thin layer of smectic A, is, using (4),

$$W_P = -\int_\Omega P u\, d\Omega = -2u_0 \frac{d}{\pi} \int_S P v\, dx dy. \tag{6}$$

The integral $I = W + W_P$ is then varied where the variations $\eta(x, y)$ satisfy $\eta = 0$ on Γ. Applying the standard variation process we obtain

$$\begin{aligned} \delta I &= \frac{1}{2} u_0^2 d \int_S \left[\overline{B}\left(\frac{\pi}{d}\right)^2 v - \frac{4P}{\pi u_0} - \chi_a H^2 \Delta v\right] \eta\, dS \\ &\quad + \frac{1}{2} u_0^2 d K_1\, \delta \int_S \left[\frac{1}{2}(\Delta v)^2 + 2(v_{xy}^2 - v_{xx}v_{yy})\right] dS. \end{aligned} \tag{7}$$

The variation of the second integral in equation (7) has been discussed in great detail in Landau and Lifshitz[8] (Chapter 2). Let $\boldsymbol{\nu}$ and $\mathbf{l}$ denote the unit outward normal to Γ and the unit tangent vector to Γ respectively and suppose that the smectic layers are simply supported[8], in the sense that η must be zero on Γ while $\partial\eta/\partial\nu$ may be arbitrary. The layers are therefore allowed to possess a 'hinge' flexibility with no displacement on Γ. For variations which vanish on Γ it can be shown that[6] (see also reference [8, p.42] with $\sigma = -1$)

$$
\begin{aligned}
&\delta\int_S \left[\frac{1}{2}(\Delta v)^2 + 2(v_{xy}^2 - v_{xx}v_{yy})\right] dS \\
&= \int_S (\Delta^2 v)\eta\, dS + \oint_\Gamma \left[\Delta v + 2(2\sin\theta\cos\theta\, v_{xy} - \sin^2\theta\, v_{xx} - \cos^2\theta\, v_{yy})\right]\frac{\partial\eta}{\partial\nu}\, dl \\
&- \oint_\Gamma \left[\frac{\partial\Delta v}{\partial n} + 2\frac{\partial}{\partial l}\left\{\sin\theta\cos\theta(v_{yy} - v_{xx}) + (\cos^2\theta - \sin^2\theta)v_{xy}\right\}\right]\eta\, dl, \quad (8)
\end{aligned}
$$

where θ is the angle between the x- axis and the outward normal $\boldsymbol{\nu}$ to Γ and $\Delta^2 = \Delta(\Delta)$ is the bi-harmonic operator. From (7) and (8) it is seen that at equilibrium, that is when $\delta I = 0$, we require in S

$$
\int_S \left[\overline{B}\left(\frac{\pi}{d}\right)^2 v - \frac{4P}{\pi u_0} - \chi_a H^2 \Delta v + K_1 \Delta^2 v\right]\eta\, dS = 0 \quad (9)
$$

and, since $\eta = 0$ and $\partial\eta/\partial\nu$ is arbitrary on Γ,

$$
\oint_\Gamma \left[\Delta v + 2(2\sin\theta\cos\theta\, v_{xy} - \sin^2\theta\, v_{xx} - \cos^2\theta\, v_{yy})\right]\frac{\partial\eta}{\partial\nu}\, dl = 0. \quad (10)
$$

Equations (9) and (10) are the governing equilibrium equations on S and Γ respectively. For the aforementioned simply supported boundary conditions the terms between the square brackets in (10) equate to zero on Γ when[8,p.44]

$$
v = 0, \qquad \text{and} \qquad \frac{\partial^2 v}{\partial\nu^2} - \frac{d\theta}{dl}\frac{\partial v}{\partial\nu} = 0. \quad (11)
$$

Equation (11) is quite general for simply supported conditions and will be applicable for any shape of domain in the xy-plane.

RECTANGULAR DOMAINS

In the rectangular geometry of Fig.1, θ is always a constant and the boundary conditions (11) become

$$
v = 0 \ \text{ on } \ \Gamma, \qquad v_{xx} = 0 \ \text{ on } \ x = 0, a, \qquad v_{yy} = 0 \ \text{ on } \ y = 0, b. \quad (12)
$$

The bulk equilibrium equation is, from equation (9),

$$
\Delta^2 v - \frac{\chi_a}{K_1}H^2\Delta v + \left(\frac{\pi}{d\lambda}\right)^2 v = \frac{4P}{\pi K_1 u_0}. \quad (13)
$$

A Navier type of solution will now be sought, following the method outlined by Timoshenko and Woinowsky-Krieger[9,p.272]. We write the constant term in (13) as the double half-range Fourier series,

$$\frac{4P}{K_1 \pi u_0} = \sum_{n=1,3,5...}^{\infty} \sum_{m=1,3,5...}^{\infty} P_{mn} \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right), \tag{14}$$

valid on the range $0 \leq x \leq a$, $0 \leq y \leq b$, with $P_{mn} = \frac{64P}{K_1 \pi^3 u_0 mn}$. This series clearly satisfies the boundary conditions in (12). The series

$$v(x, y) = \sum_{n=1,3,5...}^{\infty} \sum_{m=1,3,5...}^{\infty} A_{mn} \sin\left(\frac{m\pi x}{a}\right) \sin\left(\frac{n\pi y}{b}\right) \tag{15}$$

when inserted with (14) into (13) is a solution satisfying the boundary conditions (12) provided

$$A_{mn} = P_{mn} \left[\left(\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \right)^2 + \left(\frac{\pi}{d\lambda}\right)^2 - \frac{\chi_a}{K_1} H^2 \left(\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \right) \right]^{-1}. \tag{16}$$

The coefficient of A_{mn} becomes singular as a function of H when H satisfies

$$-\frac{\chi_a}{K_1} H^2 = \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 + \left(\frac{\pi}{d\lambda}\right)^2 \left[\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \right]^{-1}. \tag{17}$$

The right-hand side of (17) is minimized with respect to m and n when

$$\left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 = \frac{\pi}{d\lambda}. \tag{18}$$

The terms in the series with maximum amplitude are determined from the m and n which give the closest approximation to (18). Also, when (18) holds the critical value of H is found from (17) to be (recall that $\chi_a < 0$)

$$H_c = \sqrt{-2\frac{K_1}{\chi_a}\frac{\pi}{d\lambda}}. \tag{19}$$

which is the critical field result analogous to that for an infinite sample[4].

As an example we consider the values (in cgs units)

$$b = a = \pi, \quad d\lambda = \pi \times 10^{-2}, \quad K_1 = 10^{-6}, \quad \chi_a = -10^{-7}, \quad \lambda = 2 \times 10^{-7}. \tag{20}$$

These values for K_1, χ_a and λ are similar to those used in [4, p.363] where $d\lambda = 2 \times 10^{-8}$ is physically realistic; the above choice for $d\lambda$, although unphysical, will not affect the qualitative aspects of the graphs shown below

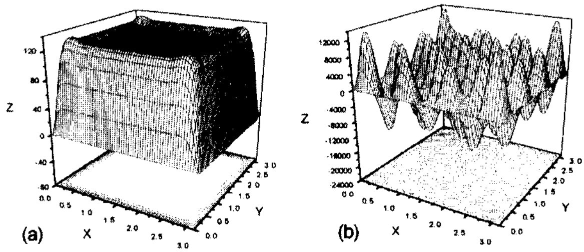

FIGURE 2 Surface and contour plots (*cgs* units) for the first ten terms in the series (15) representing the surface displacement v at the mid-plane for the physical parameters given in the text.

since decreasing $d\lambda$ increases the number of 'grids' appearing, as can be determined similarly to the following. The (odd) values of m and n which give the closest approximation to $\pi/d\lambda = 100$ are $m = n = 7$, indicating that the term involving A_{77} contains the dominant modes as H approaches H_c from below. Since (18) is not identically satisfied for these particular values, the solution is actually valid until H finally satisfies (17) for $m = n = 7$, slightly above the value given by (19). Here, $H_c = 44.7214$ while the solution actually becomes singular at $H = 44.7259$.

We examine the surface displacement around the mid-plane $z = d/2$. The sum of the first ten terms in the solution (15) with (20) is plotted for the values of $H = 0$, and $H = H_c = 44.7214$. Motivated by physical considerations, we choose $P = 1000$ (*cgs*) and set $u_0 = 10^3 \sim 10^{-2}d$ (i.e. u_0 is around 1% of depth d). Fig.2(a) shows the solution for $H = 0$ and Fig.2(b) is the solution for $H = H_c = 44.7214$. The undulations are largest near the corners in the xy-plane. At $H = H_c$ there is a two-dimensional 7×7 grid-like pattern reminiscent of that depicted in Chandrasekhar[5,p.282] for undulations induced by a magnetic field in cholesteric liquid crystals. A more physically meaningful value of $d\lambda = 2 \times 10^{-8}$ lends itself to a similar analysis: e.g. $P = 1000$, $d = 10^{-1}$, $u_0 = 10^{-3}$ gives similar plots to Fig.2 except that H_c is larger and a much greater number of grids appears as H approaches H_c.

RADIAL DOMAINS

We now consider a circular boundary where ϕ and r are the usual polar coordinates with $0 \leq \phi \leq 2\pi$, $0 \leq r \leq R$. It is not expected that the solution be ϕ dependent and attention is therefore restricted to $v = v(r)$.

Since $\Delta = r^{-1}\partial/\partial r(r\partial/\partial r)$ the equilibrium equation (13) becomes

$$\frac{\partial^4 v}{\partial r^4}+\frac{2}{r}\frac{\partial^3 v}{\partial r^3}-\frac{1}{r^2}\frac{\partial^2 v}{\partial r^2}+\frac{1}{r^3}\frac{\partial v}{\partial r}-\frac{\chi_a H^2}{K_1}\left(\frac{\partial^2 v}{\partial r^2}+\frac{1}{r}\frac{\partial v}{\partial r}\right)-\frac{4P}{\pi K_1 u_0}+\left(\frac{\pi}{d\lambda}\right)^2 v=0. \tag{21}$$

The boundary conditions (11) must also apply. We anticipate that the

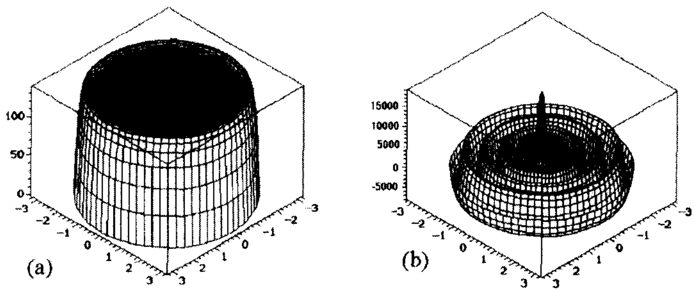

FIGURE 3 The mid-plane displacement $v(r)$ with the parameters in the text, $0\leq r\leq\pi$: (a) $H=0$, (b) $H=44.7\approx H_c$.

solution will contain Bessel functions and so we suppose that the solution is finite at $r=0$. The boundary conditions can then be written as

$$|v(r)|<\infty \quad \text{at} \quad r=0, \tag{22}$$

$$v(r)=0, \quad \frac{\partial^2 v}{\partial r^2}-\frac{1}{r}\frac{\partial v}{\partial r}=0 \quad \text{at} \quad r=R. \tag{23}$$

The general solution to (21) is, for arbitrary constants A, B, C and D,

$$v(r)=AJ_0(\beta r)+BJ_0(\gamma r)+CY_0(\beta r)+DY_0(\gamma r)+\frac{4P(d\lambda)^2}{\pi^3 K_1 u_0} \tag{24}$$

where J_0 is the Bessel function of the first kind of order zero and Y_0 is the Bessel function of the second kind of order zero and β and γ are defined by

$$\beta^2=-\frac{\chi_a H^2}{2K_1}+\sqrt{\frac{\chi_a^2 H^4}{4K_1^2}-\frac{\pi^2}{\lambda^2 d^2}}, \qquad \gamma^2=-\frac{\chi_a H^2}{2K_1}-\sqrt{\frac{\chi_a^2 H^4}{4K_1^2}-\frac{\pi^2}{\lambda^2 d^2}}. \tag{25}$$

The boundary conditions force $C=D=0$. We then use conditions (23) to find A and B by solving

$$\begin{bmatrix} J_0(\beta R) & J_0(\gamma R) \\ \frac{2\beta}{R}J_1(\beta R)-\beta^2 J_0(\beta R) & \frac{2\gamma}{R}J_1(\gamma R)-\gamma^2 J_0(\gamma R)\end{bmatrix}\begin{bmatrix} A \\ B\end{bmatrix}=\begin{bmatrix}\frac{-4P(d\lambda)^2}{\pi^3 K_1 u_0} \\ 0\end{bmatrix}, \tag{26}$$

J_1 being the Bessel function of the first kind of order 1. Solving (26) yields

$$A = \frac{-4P(d\lambda)^2}{\pi^3 K_1 u_0} \frac{\frac{2\gamma}{R} J_1(\gamma R) - \gamma^2 J_0(\gamma R)}{\det M}, \quad B = \frac{4P(d\lambda)^2}{\pi^3 K_1 u_0} \frac{\frac{2\beta}{R} J_1(\beta R) - \beta^2 J_0(\beta R)}{\det M}. \tag{27}$$

where $\det M$ is the determinant of the coefficient matrix in (26). The above Bessel functions cannot be expressed simply when β and γ are complex. Nevertheless, it can be shown[1] that the solution is real for all values of H. It is easily seen that (24) is real whenever β is real which is true whenever $H > H_c$, with H_c as defined above in equation (19). However, when $H < H_c$ it is not necessarily true that β is real: β and γ can be complex conjugates.

For clarity, we set $R = \pi$, $P = 1$ and use $u_0 = P$ to display the qualitative properties of the solution $v(r)$. Figs.3(a),(b) show $v(r)$ when $H = 0$ and $H = 44.7 \approx H_c$ (cgs units), respectively. As for the rectangular domains, more physically realistic choices for the parameters are possible: a much greater number of ridges appears as H approaches H_c.

CONCLUSIONS

A model has been developed which allows an analysis of Helfrich-Hurault layer undulations on finite domains of smectic A liquid crystals. Non-uniform pressures are currently being investigated[1], especially in respect of the apparent 'ridges' which appear near the boundaries in the above plots: recent work indicates that these effects are always present in both the domains considered above even for cases where the Fourier series methods cannot possibly display Gibbs' phenomena. The model introduced here has much to be discussed and exploited in future work.

Acknowledgements

This work was carried out while GJB held a U.K. EPSRC studentship.

References

[1] I.W. Stewart and G.J. Barclay, to appear.

[2] W. Helfrich. *J. Chem. Phys.* **55**, 839 (1971).

[3] J.P. Hurault, *J. Chem. Phys.* **59,** 2068 (1973).

[4] P.G. de Gennes and J. Prost, *The Physics of Liquid Crystals* (Clarendon, Oxford, 1993).

[5] S. Chandrasekhar, *Liquid Crystals,* 2nd ed. (CUP, Cambridge, 1992).

[6] I.W. Stewart, to appear in *Phys. Rev. E* (1998).

[7] J. Fukuda and A. Onuki, *J. Phys. II France* **5,** 1107 (1995).

[8] L.D. Landau and E.M. Lifshitz, *Theory of Elasticity,* 3rd ed. (Pergamon Press, Oxford, 1986).

[9] S. Timoshenko and S. Woinowsky-Krieger, *Theory of Plates and Shells,* 2nd ed. (McGraw-Hill, New York, 1987).