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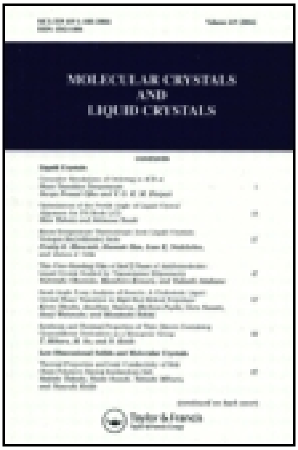

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Effects of Weak Anchoring on C1 and C2 Chevron Structures

A. Diaz [a], N. J. Mottram [a] & G. McKay [a]

[a] Department of Mathematics, University of Strathclyde, Glasgow, UK

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Effects of Weak Anchoring on C1 and C2 Chevron Structures

A. Diaz
N. J. Mottram
G. McKay
Department of Mathematics, University of Strathclyde, Glasgow, UK

We present a theoretical study of the effect of weak anchoring on the transition between C1 and C2 chevron structures in smectic C liquid crystals. We employ a continuum theory which allows for variable cone, azimuthal and layer tilt angles. Equilibrium profiles for the director cone and azimuthal angles in the C1 and C2 states are calculated from the standard Euler-Lagrange minimisation of the total energy of the system. By comparing the total energies of the C1 and C2 states we can determine the globally stable chevron profile and calculate the critical temperature for the C1–C2 transition, which depends on anchoring strength and pretilt angle variations.

Keywords: C1, C2 structure formation; surface-stabilised ferroelectric liquid crystals; weak anchoring

INTRODUCTION

Clark and Lagerwall first demonstrated the surface stabilisation of ferroelectric liquid crystals (SSFLCs) in 1980 [1] and demonstrated that it was possible to suppress the chiral helix by confining a smectic C^* material between two parallel substrates. It was soon realised that an understanding of the chevron structure of the smectic layers [2–4] was crucial to exploiting the display possibilities of SSFLCs. Since then a great deal of research has focused on the development of SSFLCs for display purposes. the chevron structure appears when a

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Address correspondence to N. J. Mottram, Department of Mathematics, University of Strathclyde, 26 Richmond Street, Glasgow G1 1XH, U.K. E-mail: nigel.mottram@strath.ac.uk

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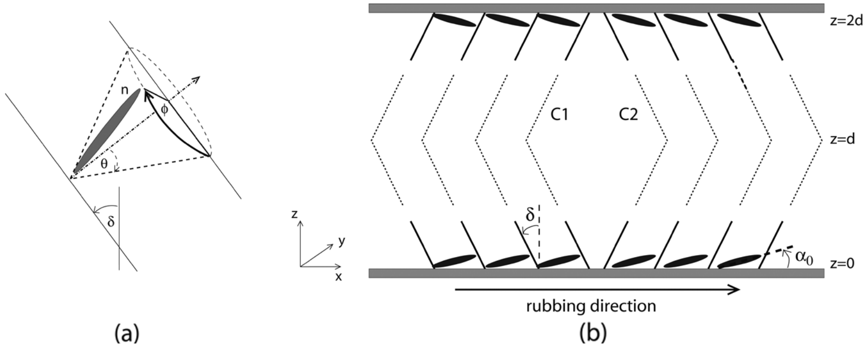

FIGURE 1 (a) Director configuration within a tilted layer illustrating the cone angle θ, azimuthal angle ϕ and layer tilt angle δ; (b) Layer configuration for C1 and C2 chevron structures.

sample of smectic A, in a bookshelf configuration, when the liquid crystal is cooled to the smectic C phase. the layer contraction that occurs during cooling is associated with a layer lengthening and thus, in a constrained system where layer continuity is conserved, layer buckling. This buckling may be degenerate so that there are two possible directions for the layer to orientate, leading to C1 and C2 chevrons (see Fig. 1). This degeneracy of the layer configuration means that different domains of the cell may be in different chevron states resulting in the formation of zigzag defects between domains [3,4]. However, when the surfaces are treated so that a specified director angle is induced ("pretilt") at the substrate, this degeneracy can be broken. Thus, one of the C1 or C2 states will be preferred leading to the removal of defects, a homogeneous device with better optical characteristics.

We will examine the effect of *weak* pretilt anchoring at the cell substrates on the formation and stability of C1 and C2 chevrons. In order to understand and predict the formation of chevrons, we examine director profiles and layer structures as the surface anchoring strength, substrate pretilt angle and sample temperature are varied.

GEOMETRY OF THE CELL

We consider a sample of smectic C liquid crystal constrained by two parallel substrates a distance $2d$ apart. We define the z-axis as the direction perpendicular to the cell substrates, the x-axis will be the rubbing direction on the substrate and the y-axis completes our orthogonal system of reference, see Figure 1. We will model the lower

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half of the cell, from $z = 0$ to $z = d$, and assume that the upper half is equivalent due to symmetry.

We can describe the smectic C phase as a layered structure where the unit director $\mathbf{n}$ makes an angle θ, the cone angle, with respect to the layer normal. The director $\mathbf{n}$ is then constrained to lie on the surface of a fictitious cone, with vertex angle 2θ. The twist angle ϕ denotes the position of $\mathbf{n}$ on the fictitious cone and the layer tilt angle δ describes the tilt of the layers from the substrate normal, see Figure 1. Using the appropriate rotation matrices, $\mathbf{n}$ can be described as

$$\mathbf{n} = \begin{bmatrix} \cos\theta(z)\cos\delta(z) + \sin\theta(z)\sin\delta(z)\cos\phi(z) \\ -\sin\theta(z)\sin\phi(z) \\ \cos\theta(z)\sin\delta(z) - \sin\theta(z)\cos\delta(z)\cos\phi(z) \end{bmatrix}. \tag{1}$$

The C1 and C2 chevrons are then characterised by, respectively, a positive or negative layer tilt angle δ in the lower half of the cell. Here, we have assumed that all angles depend only on the z-coordinate throughout the cell.

ENERGY

The liquid crystal will exhibit an equilibrium structure that attains a minimum state of the total free energy. We will consider a free energy that incorporates elasticity, thermotropic and surface anchoring effects. In the present work the following simplified elastic energy density is adopted,

$$W_{\text{elastic}} = \frac{K_\theta}{2}\left(\frac{d}{dz}\theta(z)\right)^2 + \frac{K_\delta}{2}\left(\frac{d}{dz}\delta(z)\right)^2 + \frac{K_\phi}{2}\theta(z)^2\left(\frac{d}{dz}\phi(z)\right)^2, \tag{2}$$

where K_θ, K_ϕ, and K_δ are elastic constants. Note that W_{elastic} in Eq. (2) depends only on the squares of the first derivatives of each angle, cross terms have been neglected. Also, the coefficient of the derivative of ϕ is proportional to θ^2 since (by the definition of ϕ and θ) when θ is zero, ϕ is undefined in which case gradients in ϕ should not contribute to the energy. Even though this is a simplified form of the elastic energy, the following results will be qualitatively the same if a more complicated and more accurate elastic energy [6] is used.

The thermodynamic energy density is derived from a Landau expansion of the true thermotropic energy functional in the order parameter θ [5],

$$W_{\text{therm}} = \frac{1}{2}\alpha\Delta T\theta(z)^2 + \frac{1}{4}b\theta(z)^4 + \frac{1}{6}c\theta(z)^6, \tag{3}$$

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where $\Delta T = T - T_{AC}$ is the temperature measured from the smectic A to smectic C transition temperature T_{AC}, and α, b, c are the Landau coefficients. We assume that α, b and c are temperature independent.

In this model we will also assume an empirically derived relationship [7] between the layer tilt and the cone angle, $\delta = \mu\theta$, where $|\mu| = 0.85$ is a typical experimentally determined value [7,8]. Therefore, we will model C1 and C2 chevrons by assuming $\mu = +0.85$ and $\mu = -0.85$ respectively, when $\theta > 0$.

BOUNDARY CONDITIONS

From geometrical considerations and the assumed symmetry of the chevron structure, the director is constrained to lie in the xy-plane at the chevron interface, i.e., $\mathbf{n}_3 = 0$ at $z = d$, the centre of the cell. We also assume that the cone angle $\theta(z)$ is smooth at the chevron interface [9] so that, using (1),

$$\phi(d) = \cos^{-1}\left(\frac{\tan(\delta(d))}{\tan(\theta(d))}\right), \quad \theta'(d) = 0. \tag{4}$$

At the cell substrate we allow a degree of weak anchoring. This is modelled via a Rapini-Papoular type surface anchoring [10],

$$W_{\text{surface}} = \frac{1}{2}\tau_0\left(1 - (\mathbf{n}\cdot\mathbf{n}_0)^2\right), \tag{5}$$

where τ_0 is the anchoring strength and the preferred director orientation at the substrate is

$$\mathbf{n}_0 = (\cos(\alpha_0), 0, \sin(\alpha_0)), \tag{6}$$

for a pretilt angle α_0.

By comparing $\mathbf{n_0}$ and the expression for the director $\mathbf{n}$, we observe that the preferred director angles at the substrate $z = 0$ are

$$\phi = \pi \ \text{ and } \ \theta = \frac{\alpha_0}{(1+\mu)}. \tag{7}$$

Note that the preferred cone angle θ is significantly different for C1 and C2 chevrons due to the change of sign of μ. Combining Eqs. (2), (3), and (5) we obtain the total energy per unit area in the xy-plane,

$$E = 2\left(\int_0^d (W_{\text{elastic}} + W_{\text{therm}})dz + W_{\text{surface}}|_{z=0}\right). \tag{8}$$

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NUMERICAL CALCULATIONS

The director configuration will be determined by minimisation of the total energy E of the liquid crystal layer, after non-dimensionalising via $z \to z/d$. Numerical solutions for the cone and twist angles are obtained from the Euler-Lagrange equations derived from the total energy in Eq. (8). Some examples of equilibrium profiles are shown in Figures 2 and 3. In these and subsequent figures, we have employed the following values taken from the literature [8]: $\alpha = 10^3\,\mathrm{Jm}^{-3}\mathrm{K}^{-1}$, $b = 2.1 \times 10^6\,\mathrm{Jm}^{-3}$, $c = 8.3 \times 10^6\,\mathrm{Jm}^{-3}$, $d = 3 \times 10^{-6}\,\mathrm{m}$, $K_\phi = 10^{-11}\,\mathrm{N}$, $K_\delta = 10^{-11}\,\mathrm{N}$, $K_\theta = 10^{-11}\,\mathrm{N}$. All angles shown in subsequent plots are in degrees.

Figures 2 and 3 show the cone angle $\theta(z)$ and azimuthal angle $\phi(z)$ through the cell as pretilt angle and anchoring strength are varied. We see that, in all cases, the cone angle is almost constant in the bulk of

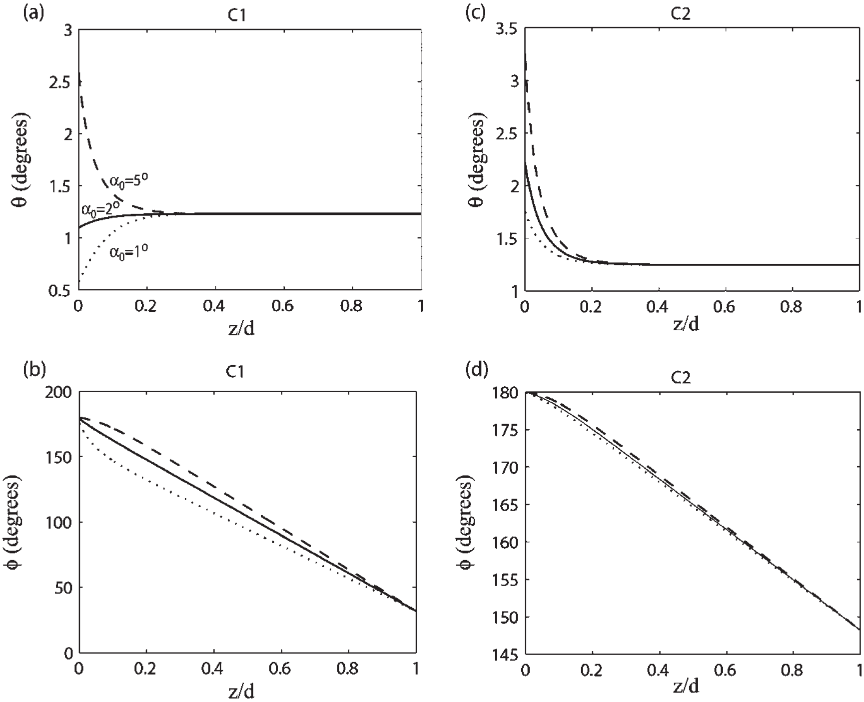

FIGURE 2 Director angles θ and ϕ profiles for the C1 and C2 chevron states as pretilt angle α_0 varies for the parameter values $\tau_0 = 10^{-3}\,\mathrm{Nm}^{-1}$ and $\Delta T = -1$. (a), (c) cone angle $\theta(z)$ for C1 and C2 respectively; (b), (d) azimuthal twist angle $\phi(z)$ for C1 and C2 respectively.

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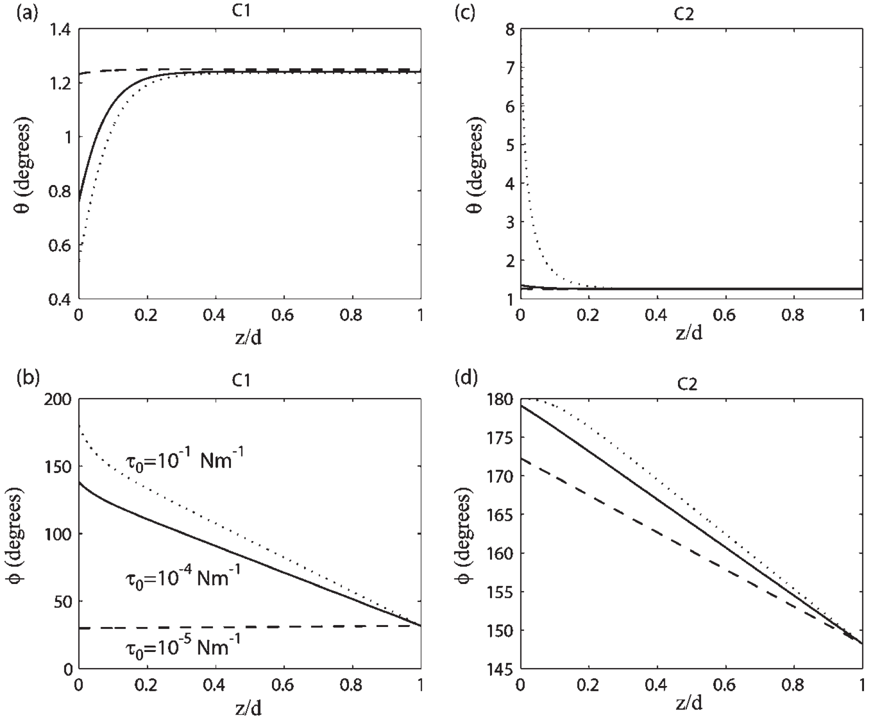

FIGURE 3 Director angles θ and ϕ profiles for the C1 and C2 chevron states as the anchoring strength τ_0 varies for the parameter values $\alpha_0 = 1^\circ$, $\Delta T = -1$. (a), (c) cone angle $\theta(z)$ for C1 and C2 respectively; (b), (d) azimuthal twist angle $\phi(z)$ for C1 and C2 respectively.

the cell at an angle θ_{eq}, the minimum of the thermodynamic energy W_{therm}. This equilibrium cone angle θ_{eq} depends only on ΔT and therefore variations of τ_0 and α_0 do not affect the θ profiles in the bulk. The graphs for $\phi(z)$ (Figs. 2(b),(d), 3(b),(d)) show a roughly linear twist of the director from the substrate value $\phi = 180^\circ$ to the chevron interface value. In the C1 case, ϕ at the chevron interface is much lower than in the C2 case, 150° in C1 and 40° in C2, due to the change of sign of μ in the chevron condition in Eq. (4).

In Figures 2 and 3, any deviation in the cone or twist angle from, respectively, a constant or linear twist profile occurs close to the substrate. In Figure 2, as the pretilt angle is varied the cone angle changes in an attempt to attain the preferred value from Eq. (7). In the C1 case, when $\mu = 0.85$, this is approximately half of α_0 whereas in the C2 case, when $\mu = -0.85$, this is around seven times

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α_0. In Figure 2(c) we see that the anchoring strength is not sufficient to achieve such a high surface cone angle.

The behaviour is different as the anchoring strength varies. In Figure 3 we see that whilst in the C2 case ϕ remains close to π at the substrate, in the C1 case ϕ reduces significantly, to the value prescribed by the chevron interface condition. This indicates that, as the anchoring strength is decreased, the anchoring in the C1 case "breaks" before the anchoring in the C2 case. In Figure 3(b), at $\tau_0 = 10^{-5}\,\mathrm{Nm}^{-1}$, the azimuthal angle at the surface is far from the preferred substrate value ($\phi(0) = 180^\circ$) but has reduced to the value at the chevron interface $\phi \approx 40^\circ$ throughout the cell in order to minimize the elastic energy. However, in Figure 3(d) at $\tau_0 = 10^{-5}\,\mathrm{Nm}^{-1}$, the azimuthal angle at the surface remains close to the preferred value. This is due to the fact that there exists high azimuthal elastic energy in the C1 state when the director twists through the large azimuthal angle from the preferred substrate angle to the chevron interface angle ($180^\circ \rightarrow 40^\circ$). In the C2 state the required twist is smaller ($180^\circ \rightarrow 150^\circ$) and thus the elastic energy is smaller.

COMPARISON OF ENERGIES

We now examine the total energy of the system, E, for the C1 and C2 states as the temperature, the substrate pretilt and anchoring strength are varied. From Figure 4 we see that the C2 state has the lower energy for small pretilt angles. As the pretilt angle increases, the C1 state lowers in energy, with a crossover at a critical pretilt. This behaviour can be explained by considering the preferred value of θ at the substrate compared to the bulk equilibrium cone angle. If we consider the energy due to the cone angle variations (the thermotropic energy and the cone angle elastic energy) we see that the minimum energy state exists when the preferred substrate cone angle value happens to coincide with the thermotropic equilibrium cone angle. (In fact, the θ dependent energy terms turn out to be the most significant energy term). The minimum energy state is then a constant cone angle $\theta(z) = \theta_{eq}$. If the preferred substrate cone angle differs from θ_{eq} there will be an associated energy increase. In the C1 state the preferred value of the cone angle at the substrate is $\alpha_0/(1 + |\mu|)$, whereas in the C2 state, when $\mu < 0$, the preferred value is $\alpha_0/(1 - |\mu|)$. For the value $|\mu| = 0.85$ the difference between these preferred values in the C1 and C2 states is significant ($0.54 \times \alpha_0$ and $6.7 \times \alpha_0$. The chevron state (C1 or C2) which has a preferred value closer to the equilibrium cone angle will be of the lowest energy.

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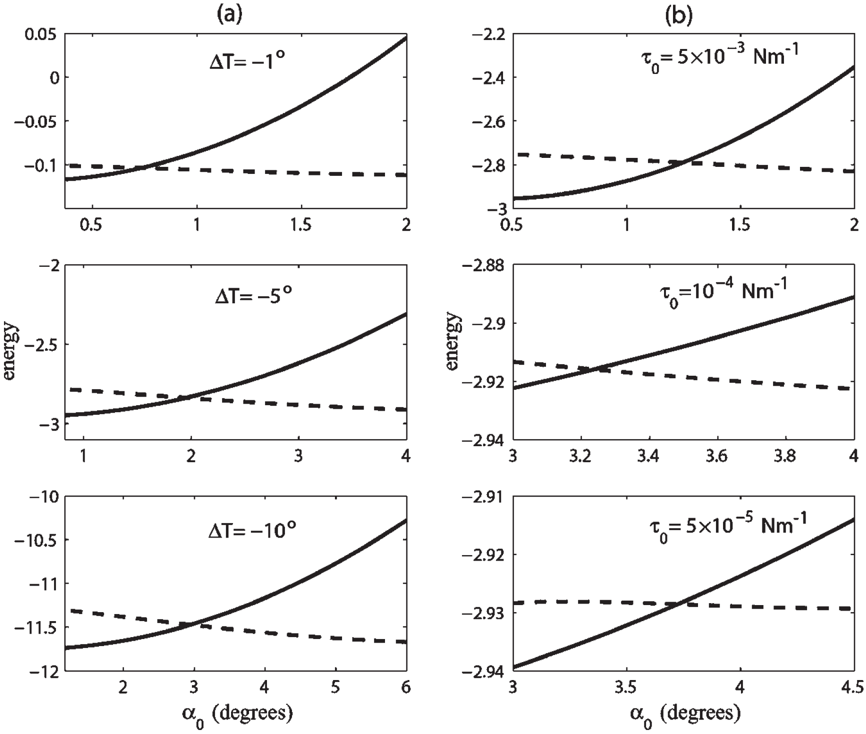

FIGURE 4 Comparison of energies for C1 and C2 chevrons as pretilt varies for: (a) different values of ΔT, with $\tau_0 = 10^{-3}\,\mathrm{Nm}^{-1}$; and (b) for different values of τ_0, with $\Delta T = -5$. Dashed lines indicate the C1 chevron energy and solid lines indicate the C2 chevron energy.

For a fixed temperature the equilibrium cone angle is fixed. For a sufficiently low pretilt value both preferred substrate cone angle values for the C1 and C2 states, $\alpha_0/(1+|\mu|)$ and $\alpha_0/(1-|\mu|)$ will be less than θ_{eq} but, since $\alpha_0/(1+|\mu|) < \alpha_0/(1-|\mu|)$, the C2 value will be closer to θ_{eq}. We therefore expect the C2 state to have a lower energy than the C1 state. This expectation is verified in Figure 4 where we see that the C2 state has lower energy at low pretilt values. As the pretilt value increases the C2 preffered cone angle $\alpha_0/(1-|\mu|)$ becomes much greater than θ_{eq} and thus the C1 state, where $\alpha_0/(1+|\mu|)$ remains close to θ_{eq}, will be of lower energy.

In Figure 4(a) we see that as ΔT decreases, and consequently θ_{eq} increases, the crossover in energy is delayed until higher values of α_0. This is clear from the above explanation since the point where $\alpha_0/(1-|\mu|) = \theta_{eq}$ will now occur at a higher value of α_0. For weaker anchoring strengths, see Figure 4(b), the director at the substrate has less of a tendency to attain the preferred value and the crossover in energies occurs only when the pretilt is relatively large.

SUMMARY

We have calculated director and chevron profiles in a smectic C liquid crystal as a function of anchoring strength, pretilt and temperature. We have found the crossover on energies between the C1 and C2 states is highly dependent on both anchoring strength and pretilt value. As anchoring strength is decreased we have demonstrated that the director anchoring breaks in the C1 state before the C2 state. We have also shown that with increased pretilt angle and increased anchoring strength the C2 state is preferred over the C1 state.

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