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Nigel J. Mottram [a] & Steve J. Elston [a]

[a] Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, U.K.

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Formation and Stability of Smectic C Chevrons

NIGEL J. MOTTRAM and STEVE J. ELSTON

Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, U.K.

We have investigated theoretically chevron formation in smectic C materials and the transformation of this chevron structure to a tilted layer structure as the cell is sheared. We find a series of transition temperatures at which the behaviour of the cell critically changes and the number of possible cell configurations increases. These structures include tilted layers, single chevrons, multiple chevrons and asymmetric chevrons. Although most of the more complex multiple chevron structures are unstable we show, using a relatively simple dynamical model, that these structures may appear transiently during the formation of the stable, single chevron structure.

Keywords: theory; smectic; chevron

INTRODUCTION

Smectic C chevrons were first discovered by Rieker et al[1] using X-ray scattering and later confirmed using guided mode techniques by Elston and Sambles[2]. Since then there has been considerable commercial interest in smectic C materials due to their potential for exploitation as display devices. Key to the development of such devices is an understanding of the chevron structure and how it switches in a surface stabilised cell.

The chevron structure is thought to form due to the need to reconcile the mismatch between the smectic layer thickness in the bulk of the cell and the prescribed smectic A ordering at the cell surfaces. As the smectic A to smectic C phase transition is crossed the increasing molecular tilt angle (the cone angle θ) results in a decrease in the smectic layer thickness. The resulting difference between the layer thickness at the surface and in the bulk, and the

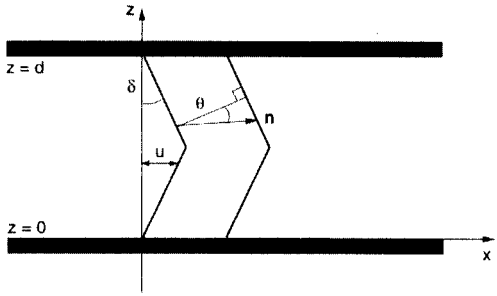

Figure 1: The cell configuration (at zero shear) indicating the director $\mathbf{n}$ which is contained within the xz-plane, the cone angle θ, the layer tilt angle δ and the layer displacement, u.

need to avoid the formation of energetically unfavourable defects, leads to a tilting of the layers thus maintaining the *effective* layer density wave throughout the cell.

It is thought that a chevron, in which the layers are tilted in opposite directions in the two halves of the the cell (see Fig. 1), is formed rather than a simple tilted layer due to a pinning of the layers at the cell surface. Recently, Cagnon and Durand[3] added weight to this argument by confiming that the smectic layer position is *frozen* in the smectic A phase at the surfaces. In this paper we will model theoretically the formation of the chevron structure and more complicated multiple chevron structures as the temperature is decreased below the smectic A to smectic C phase transition. We will also investigate the effect of shearing the cell and show that a chevron structure may be transformed into a lower energy tilted layer structure by shearing one of the cell surfaces.

THE MODEL

As previously mentioned, the main assumption of the model we use in this paper is that any change in layer thickness must be accompanied by changes in the cone angle, θ, and therefore that there is no absolute layer compression or dilation. Thus as one cools from

the smectic A phase into the smectic C phase the layer thickness decreases and, if we assume that within a cell the smectic layer number is preserved (i.e. there is no layer reorganisation or defects), there will be a tendency for the smectic A bookshelf structure to *tilt* in order to retain the layer packing density wave. If the liquid crystal is strongly anchored at the surfaces this leads to the formation of a chevron consisting of regions of equal and opposite layer tilt. The chevron interface, between these two regions of opposite tilt, is assumed to be a localised bend of the layers as opposed to the discontinuous kink of the original model of Clark et al[4].

In order to simplify the calculations we also assume that the azimuthal director angle is constant and that the director always lies in a plane perpendicular to the cell surfaces (see Fig. 1). We therefore restrict ourselves to considering *planar* chevrons, previously discussed by Vaupotič et al[5] and the present authors[6]

These assumptions directly imply the condition that the layer tilt, δ, is zero at the chevron interface. In order to preserve the layer packing density wave this also means that the liquid crystal will be in the smectic A phase at the chevron interface.

This simplified model is intended to show qualitatively the effect of shearing smectic chevrons. Clearly the chevrons contained within ferroelectric display devices are necessarily non-planar since the two possible chevron interface configurations produce the essential bistability of the device (in the C2 configuration) and whilst the regime of planar chevrons is small their behaviour under shear may be indicative of the behaviour of non-planar chevrons. It is also worth noting that, although in this paper we will concentrate on smectic C chevron behaviour due to their importance in display technology, the assumption that the director remains in the plane of the chevron implies that this model will also be applicable to the formation of smectic A chevrons.

The structure of the chevron will be governed by a balance of forces due to deviations of the cone angle from it's equilibrium bulk value and elastic forces due to distortions of the director field. For small cone angles the energy (per unit area) due to the former may be written in terms of a Landau-de Gennes expansion in even

powers of θ (due to the symmetry, $\theta \leftrightarrow -\theta$) and the latter as the Frank nematic energy of distortions within a layer,

$$F = \int_0^d f_0 + \frac{a}{2}\theta^2 + \frac{b}{4}\theta^4 + \frac{K}{2}\left((\nabla.\mathbf{n})^2 + (\nabla \wedge \mathbf{n})^2\right)\mathrm{d}z, \qquad (1)$$

where $a = \alpha(T - T_{AC})$ and T_{AC} is the smectic A to C transition temperature and K is an elastic constant. In eq. (1) f_0 is the free energy in the undistorted smectic A phase i.e. when $\theta = 0$ and $\mathbf{n} = (1, 0, 0)$. Any constant energy term such as f_0 will not enter the minimization of the free energy and will subsequently be disregarded. The Landau-de Gennes energy terms in eq. (1) determine the bulk cone angle. Minimization of eq. (1) with $\mathbf{n} = (1, 0, 0)$ leads to the solutions $\theta = 0, \pm\theta_e$ where $\theta_e = \sqrt{\frac{-a}{b}}$. Thus in an undistorted sample of smectic material the cone angle will be zero for temperatures above the transition temperature T_{AC} (i.e. $a > 0$) and non-zero for temperatures below T_{AC} (i.e. $a < 0$). The equilibrium cone angle is thus directly related to the temperature by $\theta_e = \sqrt{\alpha(T_{AC} - T)/b}$.

If the director remains in the xz-plane the director $\mathbf{n}$ may be written as (Fig. 1) $\mathbf{n} = (\cos(\delta - \theta),\ 0,\ \sin(\delta - \theta))$ and if we assume that the layer tilt angle, δ, and the smectic cone angle, θ, are small and that there is a direct relationship between them, $\delta = \nu\theta$ the free energy reduces to,

$$F = \int_0^d \frac{b}{4}\left(\theta^2 - \theta_e^2\right)^2 + \frac{K'}{2}\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 \mathrm{d}z, \qquad (2)$$

where $K' = K(1 - \nu)^2$. This relationship between δ and θ may be used to describe rod-shaped liquid crystal molecules for which $\nu = 1$ or, the more realistic, ellipse-shaped liquid crystal molecules for which $\nu < 1$[7].

In order to find the equilibrium configuration, the free energy must be minimized subject to certain constraints at the cell surfaces. The first boundary conditions are related to the induced ordering at the cell surfaces. If we assume that the liquid crystal is strongly anchored in the direction of the layer normal at the cell surfaces this implies that the cone angle, θ, is equal to the layer tilt angle,

δ, there. For $\nu \neq 1$, this will only occur in the smectic A phase i.e. when $\theta = 0$ and the boundary conditions are therefore $\theta = 0$ on $z = 0,\ d$.

We also wish to include a parameter which measures the total amount of shear between the two surfaces. If we assume that the lower surface is fixed and the upper is sheared by an amount τ then the amount of shear is related to the smectic layer configuration by,

$$\tau = \int_0^d \nu\theta \mathrm{d}z. \tag{3}$$

We now have the full equilibrium problem. We must determine the chevron structure, $\theta(z)$, which minimizes the free energy (2) subject to the boundary conditions $\theta = 0$ on $z = 0,\ d$ and the constraint (3). We can simplify the system by nondimensionalising all variables. By introducing the scaled coordinate $Z = z/d$ and introducing the parameters $B = bd^2/K'$, and $\eta = \tau/(d\nu)$ the system may be described in terms of the following three parameters; B, the ratio of energy terms associated with changes in the cone angle and distortions of the director, θ_e, the equilibrium bulk cone angle and η, the normalised shear. If we assume the material constant B is largely independent of temperature then our two control parameters will be θ_e and η, changes of which correspond to changes in temperature and shear respectively.

In order to model the non-equilibrium, dynamics of the formation of chevrons we will use a time dependent Landau-Ginzburg equation,

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}Z^2} - B\theta\left(\theta^2 - \theta_e^2\right) = \frac{\mathrm{d}\theta}{\mathrm{d}T}, \tag{4}$$

where $T = t/\mu$ is time scaled with the effective viscosity of layer tilting. This equation, which is solved with the same shear constraint and boundary conditions as the equilibrium problem, indicates that the rate of change of the tilt angle is proportional to the gradient of the energy surface (2) and has previously been studied in relation to chevron formation by Shalaginov et al[8] where a more in depth discussion as to it's derivation may be found. We will show in this paper that even though certain complex structures are unstable they

may appear transiently during the formation of the single chevron structure.

NUMERICAL SOLUTIONS

In order to solve the equilibrium problem we use the numerical continuation package AUTO97[9] which allows us not only to find the equilibrium configuration, but examine the behaviour of the system as a parameter is varied continuously. We have thus selected three temperatures which indicate the behaviour of the system and allow the shear parameter to vary continuously. Using the typical parameter values[10], $K = 10^{-11}$N, $\alpha = 1.7 \times 10^2 \mathrm{Nm}^{-2}/\mathrm{K}$, $b = 4.1 \times 10^4 \mathrm{Nm}^{-2}$, $\nu = 0.85$ and $d = 10^{-6}$m the third parameter is found to be $B = 1.822 \times 10^5$.

Figure 2 shows the numerical results as the nondimensionalised shear, η, is varied when $\theta_e = 0.01,\ 0.02,\ 0.035$. For each value of θ_e the free energy of the system, F, is plotted as η varies. At each value of θ_e we have also plotted the cone angle $\theta(Z)$ and the nondimensionalised layer displacement $U(Z) = u(Z)/(d\nu)$ for various values of η on the solution branch. In these figures solid and dashed lines indicate stable and unstable solutions respectively.

We find that there exists a critical value $\theta_e^{(1)} = 0.00736$ at which the system changes. For $\theta_e < 0.00736$ the bookshelf configuration is stable and is the minimum energy configuration with respect to changes in the value of the shear η. If the cell is sheared the free energy increases and the bookshelf continuously transforms into a tilted layer. In order to preserve the layer density wave the layer tilting is accompanied by an increase in the value of the cone angle in the cell. The smectic A ordering at the surface leads to boundary layers at $z = 0$ and d where the layer tilt induced by shear realigns to ensure that $\delta = 0$ (and $\theta = 0$) at the surface. In this tilted layer situation it is only at the surfaces that the material is smectic A wheras the interior of the cell is smectic C.

For $\theta_e > 0.00736$ the bookshelf structure is no longer the minimum energy configuration for all shear values (Fig. 2(a)). There now exist two symmetric states with non-zero values of η which

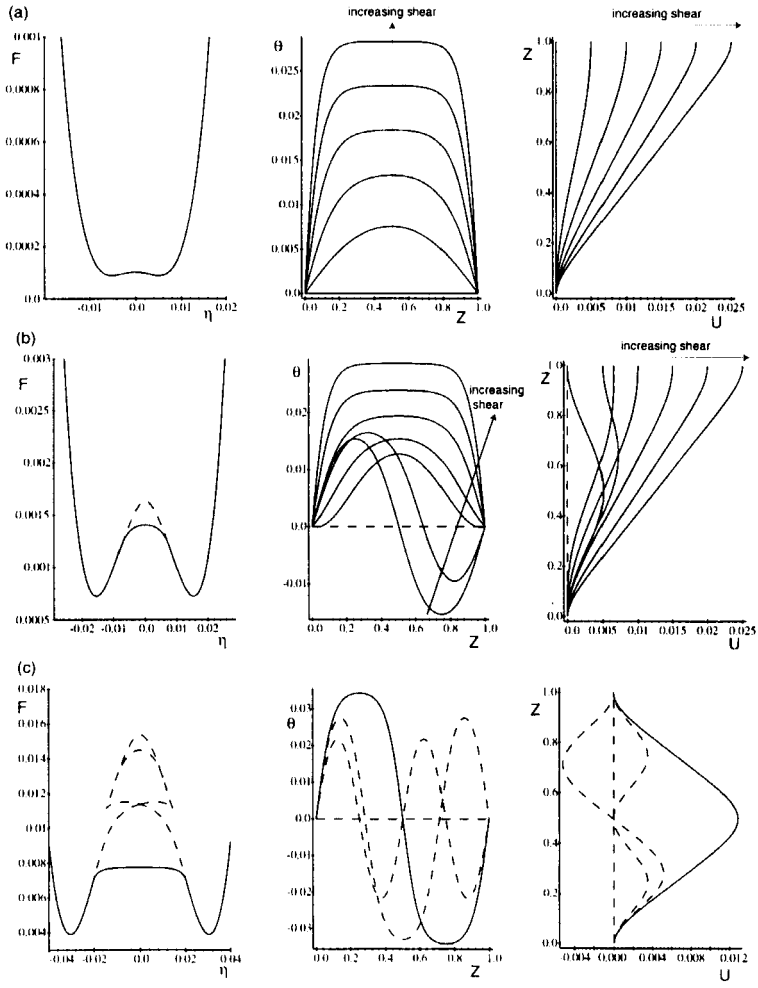

Figure 2: Numerical solutions for (a) $\theta_e = 0.01$, (b) $\theta_e = 0.02$ and (c) $\theta_e = 0.035$. From left to right the plots for each value of θ_e are; the free energy F, versus nondimensionalised shear η, the cone angle $\theta(Z)$ through the cell and the nondimensionalised layer displacement $U(Z)$ through the cell.

are the global energy minimizers corresponding to tilted layers. It should be noted that for $\eta = 0$ the bookshelf structure *is* the stable configuration. It is only if the cell is sheared or free to shear that it reaches its minimum energy configuration. The $\theta(Z)$ and $U(Z)$ plots show that the bookshelf structure continuously transforms into a tilted layer structure as η increases.

The next change in the system occurs at the critical value $\theta_e^{(2)} = 0.01472$. For $\theta_e > 0.01472$ the bookshelf structure destabilises. As θ_e increases past $\theta_e^{(2)}$ a second solution branch forms (at $\eta = 0$) with a lower energy than the bookshelf branch. This is the (single) chevron solution branch. Thus in Fig. 2(b) the lower energy, stable branch at $\eta = 0$ corresponds to the chevron solution whilst the higher energy, unstable branch corresponds to the bookshelf solution. The $\theta(Z)$ and $U(Z)$ plots in Fig. 2(b) show the unstable bookshelf solution ($\theta(Z) = 0$, $U(Z) = 0$), the stable chevron solution and how this chevron is continuously transformed to the tilted layer as η is increased. We see that the chevron interface, which lies in the centre of the cell when $\eta = 0$, moves towards the upper cell surface forming an asymmetric chevron as the cell is sheared and eventually combines with the surface boundary layer forming the tilted layer. The point where the bookshelf/tilted layer branch meets the chevron branch is the point where the chevron interface region meets the surface boundary layer region (at approximately $\eta = 0.0075$).

For larger values of θ_e the structure above the stable chevron branch becomes increasingly more complicated as more complex structures appear. Figure 2(c) shows the solution when $\theta_e = 0.035$. We see that for zero shear there are now four solutions (and the corresponding symmetry solutions, $Z \to 1 - Z$). As well the unstable high energy bookshelf solution and the stable low energy single chevron solution there are now *multiple chevron* solutions characterised by more than one chevron interface. At lower temperatures or higher values of θ_e more complex higher order chevrons exist.

Although these multiple chevrons are unstable solutions to the governing equations they can be observed transiently as the system relaxes from the unstable bookshelf to the stable single chevron. We

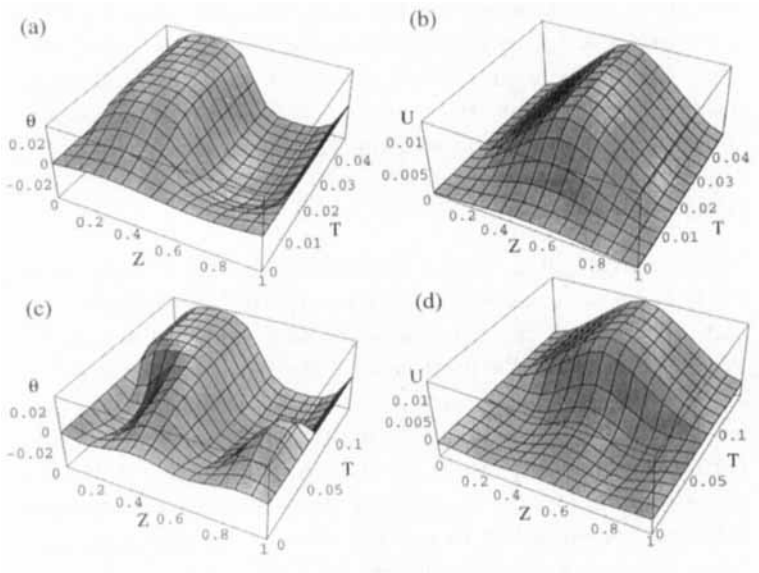

Figure 3: Formation of the single chevron structure for $\theta_e = 0.035$ and two different initial perturbations of the bookshelf structure. (a), (b) The cone angle $\theta(Z,\ T)$ and layer tilt, $U(Z,\ T)$ for the initial perturbation $\theta = 0.0035\sin(2\pi Z)$. (c), (d) The cone angle $\theta(Z,\ T)$ and layer tilt, $U(Z,\ T)$ for the initial perturbation $\theta = 0.0035\sin(4\pi Z)$.

can model this relaxation using the dynamical approach described in the previous section. Figure 3 shows the result of starting with a smectic A bookshelf structure at a temperature below the smectic A to C phase transition. Alternatively this can be thought of as quickly cooling the cell from the smectic A phase into the smectic C phase and observing the relaxation of the bookshelf structure. We have thus set the value of $\theta_e = 0.035$, the initial configuration to be the bookshelf structure ($\theta = 0$, $U = 0$) and solved eq. 4.

In Figs. 3(a) and (b) the bookshelf structure is perturbed such that at $T = 0$ the cell configuration is $\theta = 0.0035\sin(2\pi Z)$ (an order of magnitude smaller than the final configuration). This perturba-

tion grows and the single chevron state is formed. However if the same system is started with a perturbation $\theta = 0.0035 \sin(4\pi Z)$ the triple chevron structure initially grows and then later transforms into the single chevron structure, Figs. 3(c) and (d). Consequently the formation of the stable structure takes significantly longer.

DISCUSSION

We have investigated chevron formation in smectic C materials as the temperature is decreased below the transition temperature T_{AC} and the formation of a tilted layer structure as the cell is sheared. We find that below a critical value of the bulk cone angle, $\theta_e^{(2)} = 0.01472$, the bookshelf structure is stable for zero shear. It is only for cone angles greater than $\theta_e^{(2)}$ that the chevron structure forms. For larger values of θ_e, whilst the chevron structure is still the only stable solution for $\eta = 0$, there may be a large array of unstable solutions, corresponding to multiple chevrons, at higher energies. These solutions are important if the liquid crystal is quickly cooled from the smectic A phase into the smectic C phase. Starting from the unstable, bookshelf structure the system may transform into the stable, single chevron structure through an intermediate, multiple chevron structure whilst maintaining zero shear.

For non-zero shear a tilted layer structure is the global energy minimizer for cone angles greater than $\theta_e^{(1)} = 0.00736$. The smectic liquid crystal thus exerts a shear force on the upper surface. If the upper surface was free to move it would therefore move in order that tilted layers were formed within the cell.

This surface shear force, exerted by the liquid crystal is expected to be apparent if an equivalent experiment to that of Cagnon and Durand[3] was carried out on smectic C materials.

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