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# Stability of the formation of the chevron structure

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A simple model of the formation of the chevron structure and tilted layer structure in the smectic C liquid crystal phase from the bookshelf structure in the smectic A phase is considered. Energetic considerations of this system indicate that in the absence of layer pinning forces at the surface, a transition to the tilted structure is expected. However, combining the model with 'weak' surface positional anchoring effects allows the chevron structure to form.



## 1. Introduction

Chevron structures in liquid crystal cells filled with tilted smectic material were discovered by Rieker *et al.* using X-ray scattering techniques [1]. Their existence was confirmed by the discovery of a pinned point in the centre of a device by Elston and Sambles using guided mode techniques [2]. The conventional argument for chevron formation asserts that the chevron structure comes about due to the need to avoid the formation of defects and therefore satisfy the curl constraint ($\nabla \wedge \mathbf{a} = 0$, where $\mathbf{a}$ is the smectic layer normal vector) while reconciling the mismatch between the smectic layer spacing in the cell surface plane and the layer thickness in the bulk. When crossing the smectic A to smectic C phase transition, an increasing molecular tilt angle (cone angle $\theta$) results in a corresponding decrease of the smectic layer thickness. The resulting mismatch between the layer thickness values at the surfaces and within the bulk was explained in terms of the formation of structures known as chevrons. Recently Cagnon and Durand added weight to this argument when they showed that the smectic layer positioning is 'frozen' in the smectic A phase at the cell surfaces [3].

The above argument would seem to imply that the formation of a symmetric chevron structure within a surface stabilized ferroelectric liquid crystal (SSFLC) cell was inevitable. However, this is not always seen to be the case. Tilted layers are observed in the smectic C phase as are asymmetric chevrons, where the chevron tip is not midway between the two cell surfaces [4]. In fact, it is not very clear what decides whether a tilted layer structure will form in preference to a chevron within a particular cell as the SmC phase is entered. In this paper we consider a simple model of the chevron structure which allows us to investigate the relation between the chevron and tilted layer structures.

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## 2. The model

Here we make the assumption that any changes in the smectic cone angle must be accompanied by changes in the smectic layer tilt angle and therefore that there is no absolute layer compression/dilation. The only allowable change in layer thickness is that accompanied by changes in the cone angle, $\theta$. Thus, the natural or equilibrium layer thickness decreases as one cools the material from the smectic A into the smectic C phase. If we assume that within a cell the smectic layer number is strictly preserved (i.e. no reorganization of layers and no defects in the layering), and also that the layers start from a perfect bookshelf structure in the smectic A phase, i.e. they start out being perpendicular to the cell surfaces (as is commonly the case for SSFLC), the above assumptions lead to a tendency for the layers to tilt in order to retain the layer packing density wave.

As illustrated in figure 1 a number of possible smectic layer structures are consistent with this. Figure 1 (*a*) shows the simplest of these, a tilted layer structure. For this to form, the layers would have to 'slip' along the cell surfaces (on one side of the device at least). Figure 1 (*b*) shows the symmetric chevron structure. This structure is commonly, though not exclusively, observed in smectic C liquid crystal cells. For this to form, a layer kink (or localized bend) must form as the smectic A to smectic C phase transition is crossed. Figure 1 (*c*) illustrates the less frequently observed asymmetric chevron structure, which is thought to be less common due to the smectic layer slip required at the surface. It is evident that this can be viewed as being a combination of (or state between) the cases shown in figures 1 (*a*) and 1 (*b*). Finally, figure 1 (*d*) shows a multiple kinked structure (or multiple chevron). The presence of more

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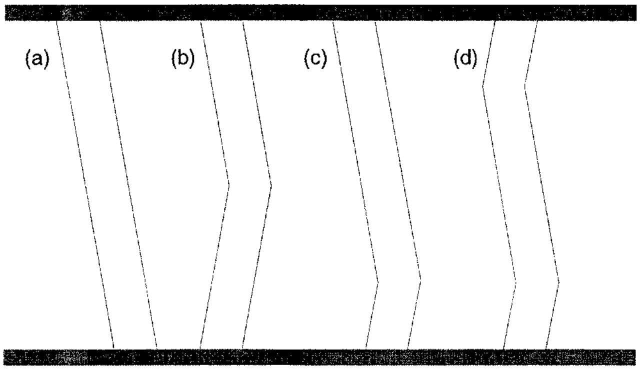


Figure 1. Structures which could form when the layers tilt in a smectic liquid crystal cell. (*a*) A simple tilted layer structure; (*b*) a symmetric chevron structure; (*c*) an asymmetric chevron structure; (*d*) a multiple chevron structure.

than one energetically expensive kink is thought to cost too much energy for this to be a stable structure, and we will not consider it further here, but will discuss it in detail in a future publication.

We can see that the structures shown in figures 1 (*a*) and 1 (*b*) can evolve into each other by passing through stages like that in figure 1 (*c*). There is an alternative, namely, that one 'arm' of the chevron reorients itself. This would however require a bulk change in the smectic layer thickness, which is highly unlikely, and so we discard it as a possible mechanism for the transition between the two structures.

In order to model these structures and the relation between them, we need some way of modelling the energetics of the chevron cusp, and of layer slippage. In the next section we present the former.



### 3. Chevron cusp and surface structure

There have been a number of models advanced to describe the chevron structure, and we use the simplest of these which keeps the director in the plane of the smectic layer normal. The following assumptions are made in our model:

(1) The chevron cusp is assumed to be a localized bend in the layering structure, as opposed to the discontinuous kink of the original Clark and Rieker model [5]. This is a necessary assumption due to the simple model of the chevron structure we are using. As the director is kept in the plane of the smectic layer normal, a kink in the smectic layer structure is not allowed because it would violate the local director continuity.

(2) At the chevron cusp, the bend is mediated through a reduction in the cone angle, $\theta$, to zero, due to layer dilation forces.

(3) The surface alignment is retained in the SmC phase.

(4) The director remains in the plane of the alignment direction.

This means that the layer structure at the cell surfaces within a SSFLC cell in the SmC phase is the same as that at the chevron cusp. The chevron cusp behaves, in effect, as an internal surface. While at first these may seem to be somewhat over-constraining assumptions, they do allow an elegant solution to the problem. Further, they are not entirely unphysical. Observation of switching in chiral smectic C liquid crystal devices shows that the chevron cusp can behave as an internal surface, and it is reasonable to assume that the smectic layer structure here is similar to that at the physical surfaces of a device. The structure of the chevron cusp is then taken to be governed by a balance of elastic forces due to distortions of the director field, and forces brought about by deviations of the cone angle from its equilibrium value in the bulk. As is conventional, we use a one constant approximation when describing the former. The free energy density due to the latter is expressed in terms of a Landau expansion in even powers of $\theta$, neglecting terms of $O(\theta^6)$ [6]. This gives a free energy density, $f$, expression.

$$f = f_0 + \frac{a}{2}\theta^2 + \frac{b}{4}\theta^4 + \frac{K}{2}[(\nabla \cdot \mathbf{n})^2 + (\nabla \wedge \mathbf{n})^2]. \quad (1)$$

This can be simplified in two ways. Firstly, as noted above, we assume that the director distortion occurs in the plane of the smectic layer normal. This allows the director distortion term to be reduced from

$$f^{\mathrm{elas}} = \frac{K}{2}[(\nabla \cdot \mathbf{n})^2 + (\nabla \wedge \mathbf{n})^2] \quad (2)$$

to

$$f^{\mathrm{elas}} = \frac{K}{2}\left(\frac{\partial \psi}{\partial z}\right)^2 \quad (3)$$

where $\psi$ is the director tilt angle. Furthermore, for small layer and director tilt angles, we can write

$$\psi \approx \frac{\theta}{\sqrt{A}} \quad (4)$$

where

$$\sqrt{A} = \left(1 - \frac{\delta_0}{\theta_0}\right)^{-1} \quad (5)$$

where $\delta_0/\theta_0$ is the ratio of smectic layer tilt to smectic cone angle in equilibrium. Secondly, the Landau terms can be conveniently re-expressed in terms of the equilibrium cone angle, $\theta_e$,

$$f^{\mathrm{LdG}} = f'_0 + \frac{b}{4}(\theta^2 - \theta_e^2)^2 \quad (6)$$

where $f_0' = f_0 - b\theta_e^4/4$, and equation (6) is obtained by minimizing the Landau term when $\theta = \theta_e$. This allows us to work with the natural (and easily observed) $\theta_e$ as a parameter, where $\theta_e$ is the equilibrium director tilt angle within the cell, at a given temperature, $T$, in the SmC phase. Thus, we can write the free energy density as,

$$f = f_0' + \frac{K}{2A}\left(\frac{\partial \theta}{\partial z}\right)^2 + \frac{b}{4}(\theta^2 - \theta_e^2)^2. \quad (7)$$

Minimizing this is equivalent to solving the relevant Euler–Lagrange equation:

$$\frac{K}{A}\left(\frac{\partial^2 \theta}{\partial z^2}\right) - b\theta(\theta^2 - \theta_e^2) = 0. \quad (8)$$

The boundary conditions require that $\theta$ is zero at the cell surfaces and the chevron interface, and defining $z = 0$ at one surface and $z = d$ at the other gives

$$\theta|_{0,d} = \theta|_{d/2} = 0. \quad (9)$$

In order to model the asymmetric chevron and tilted layer formation process, the analysis of equation (7) has to be modified to include some parameter measuring the position of the chevron cusp. This is most easily done by including a constraint that fixes the total layer displacement across the thickness of the cell.

As we have assumed for simplicity that it is valid to use small angle approximations for $\theta$ and $\delta$, we can write $(\tan \delta) \approx \delta \propto \theta$. We can then build in a constraint that

$$\int_0^d \tan \delta \, dz = \text{total layer displacement}. \quad (10)$$

This is equivalent to a constraint on the integral of $\theta$ over the thickness of the cell

$$\int_0^d \theta \, dz = \text{constant} \quad (11)$$

and can be included by adding a Lagrange multiplier term to equation (7) of the form $\lambda\theta$. This then leads to a modified Euler–Lagrange equation of the form

$$\frac{K}{A}\left(\frac{\partial^2 \theta}{\partial z^2}\right) - b\theta(\theta^2 - \theta_e^2) + \lambda = 0. \quad (12)$$

The solution of this equation is then required under the boundary conditions of equation (9).

## 4. Structure formation near the SmA–SmC phase transition

We start by considering the stability of the bookshelf structure to the formation of tilted layers of chevrons near the smectic A to smectic C phase transition. This allows us to set $\lambda = 0$ (for the bookshelf structure), and we can also assume that in the vicinity of the phase transition the actual cone angle is small, i.e.

$$\theta^2 \ll \theta_e^2. \quad (13)$$

This allows equation (8) to be rewritten as,

$$\frac{K}{A}\left(\frac{\partial^2 \theta}{\partial z^2}\right) + b\theta_e^2\theta = 0. \quad (14)$$

Further we assume that the distortion of smectic layers has two fundamental modes, corresponding to the possibilities of tilted layer structures and chevron structures, respectively, given by

$$\theta = \theta_o \sin\left(\pi \frac{z}{d}\right) \quad (15)$$

for tilted layers, and

$$\theta = \theta_o \sin\left(2\pi \frac{z}{d}\right) \quad (16)$$

for the chevron structure. We can now estimate threshold values for $\theta_e$ that govern the formation of these structures. These are given by:

$$\theta_e^{\text{tilt}} = \frac{\pi}{d}\left(\frac{K}{Ab}\right)^{1/2} = 0.00736 \quad (17)$$

for the tilted layer case, and

$$\theta_e^{\text{chev}} = \frac{2\pi}{d}\left(\frac{K}{Ab}\right)^{1/2} = 0.01472 \quad (18)$$

for the chevron case. The numerical values are for the suggested parameters of $d = 1$ µm, $K = 10^{-11}$ N, $A = 400/9$ and $b = 4.1 \times 10^4$ N m$^{-2}$ [7]. These threshold values determine the boundaries that separate different types of behaviour. There are three such regimes. Firstly, for $\theta_e < \theta_e^{\text{ilt}}$, the only energetically stable structure consists of untilted uniform layers, commonly referred to as the 'bookshelf' structure. A horizontal shear can force the smectic layering to tilt, but this will be at the cost of an increase in the energy of the system. Using a numerical solution to equation (12) this is illustrated in figure 2(*a*) using the dashed line to represent the case when $\theta_e = 0.0$ rad.

For equilibrium tilt angles in the range $\theta_e^{\text{ilt}} < \theta_e < \theta_e^{\text{hev}}$, the bookshelf structure again occurs under the constraint of zero net layer displacement. However, in this case a total displacement imposed on the layers results in a reduction in the energy of the system. This is because the tilted layer configuration has a lower energy than the uniform untilted bookshelf structure. The dashed line in figure 2(*b*) shows this for the case when $\theta_e = 0.01$ rad.

When $\theta_e > \theta_e^{\text{hev}}$, the lowest energy zero displacement structure is the chevron type structure. This means that the bookshelf structure is unstable to perturbations

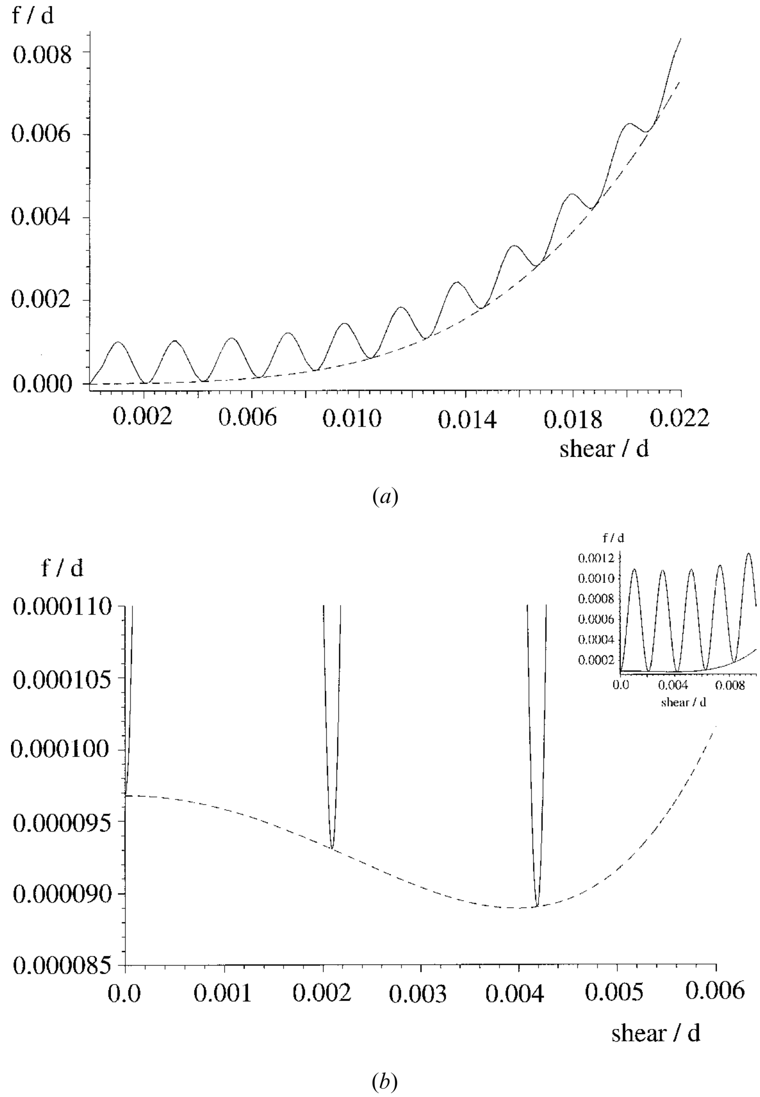


Figure 2. (*a*) The energy as a function of total displacement for the limiting case of a very small smectic tilt angle ($\theta_e = 0.0$). The dashed line shows the case without any layer positional anchoring energy and the continuous line includes such an effect as discussed in the text.



which retain zero total displacement across the cell, and under this constraint the chevron structure forms. Once again, if a horizontal shearing displacement is applied to the structure, the resulting tilted layer structure has a lower energy. For example, in figure 3 we show the case for a larger cone angle ($\theta_e \sim 0.025$ rad), corresponding to a temperature a little below $T_{AC}$. Figure 3(*a*) shows the evolution of the smectic tilt angle profile (cone angle) as the total displacement is increased, and the corresponding layer structures are shown in figure 3(*b*), where the evolution from a chevron structure to a tilted structure is clear. The total energy as a function of displacement is shown in figure 3(*c*). It should be noted that the slope of the energy–displacement curve is always zero for chevron cusps that are situated in the centre of the cell, indicating that this symmetric structure is indeed at a stationary point (as we would intuitively expect). This is because the energy is symmetric for displacements of the layers about this point.

For a typical cell thickness of 1 μm and, for example, a smectic cone angle of 0.05 rad, the behaviour is shown in figure 4. The energy density used in the model, equation (7), can be integrated to give a chevron energy $E \sim 0.01132 \times 10^{-6}$ N m$^{-1}$. For the tilted layer structure we get $E \sim 0.02264 \times 10^{-6}$ N m$^{-1}$. It should be noted that for both these cases, the same parameters have been used as in the above analysis. We can also see in figure 4(*c*) that the energy is approximately constant for a wide range (for this case, ~0.02 μm) of displacements. This region corresponds to the case of asymmetric chevrons where the bend in the layers, corresponding to the chevron cusp in our model, does not extend out to either of the cell surfaces. However, for the case where the cusp has been displaced far enough to come within

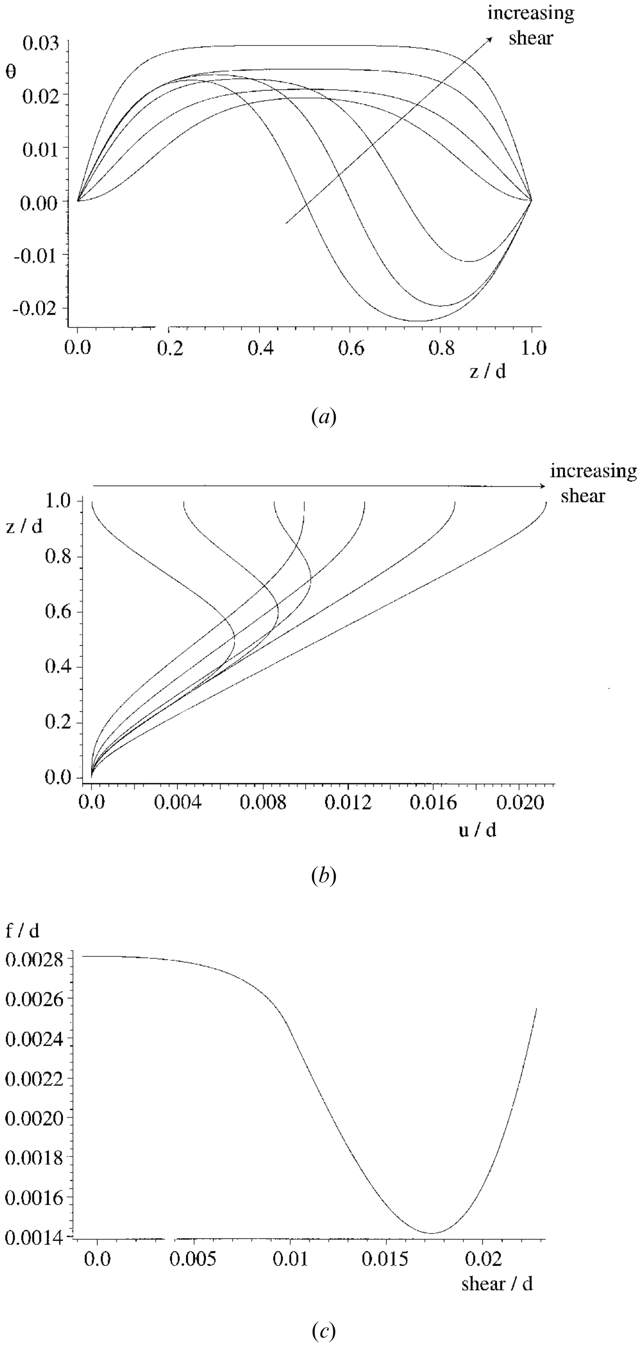


Figure 3. For a smectic tilt angle of $\theta_e = 0.025$ rad, the equilibrium chevron structure at zero displacement is increased. As this occurs, the tilt angle profiles evolve as shown in (*a*), the layer structure evolves as shown in (*b*), and the energy evolves as shown in (*c*).

a correlation length of the cell surfaces, the energy rapidly falls off to the value for a tilted layer structure, as the chevron cusp merges with the cell surface to produce a tilted layer structure.

We can also obtain an analytic solution in the region of the chevron cusp and surfaces, which in this case

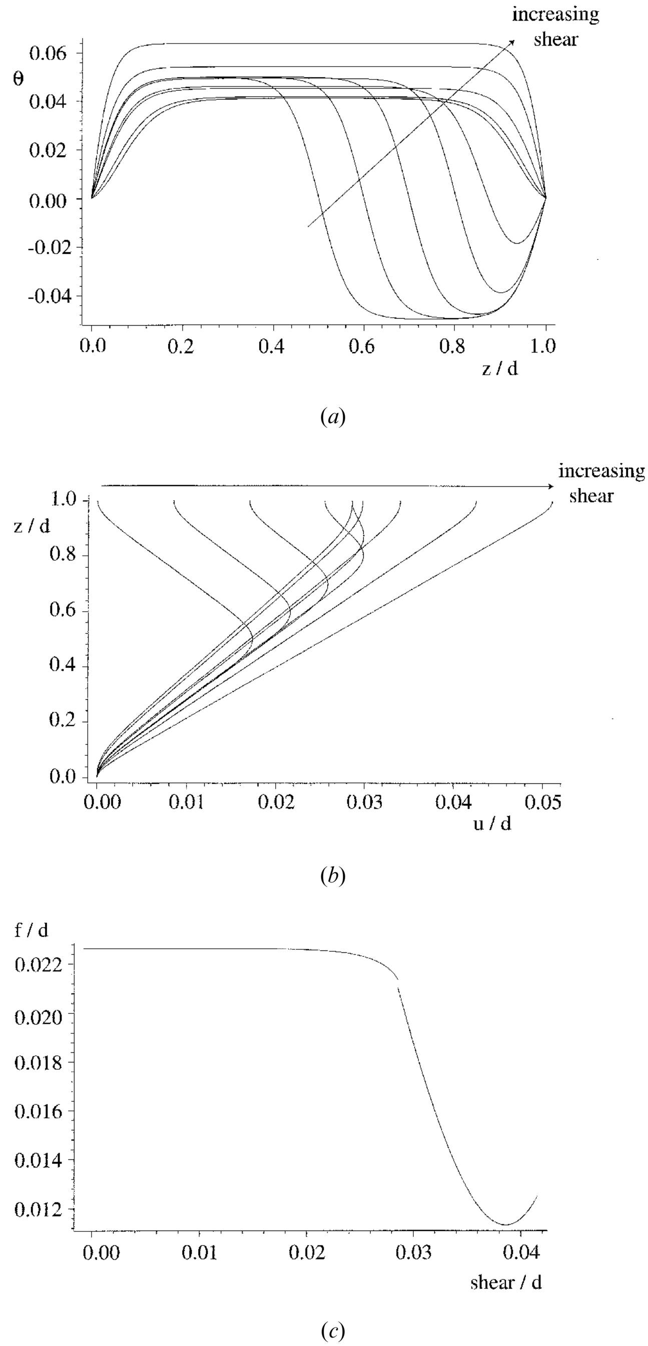


Figure 4. The evolution of (*a*) the tilt angle profile, (*b*) the layer structure and (*c*) the energy as the total displacement is increased for a smectic tilt angle of $\theta_e = 0.05$ rad. Note the appearance of a first order transition in the energy—this will be discussed in detail in a further publication.

leads to the following:

$$\theta = \theta_e \tanh\left[\left(\frac{\theta_e^2 bA}{2K}\right)^{1/2} z\right] \tag{19}$$

where, for each case, $z$ is measured away from the $\theta = 0$ point.

To obtain the energy of the chevron cusp, we substitute equation (19) back into equation (7) to get:

$$f - f_0' = \frac{1}{2} b\theta_e^4 \operatorname{sech}^4\left[\left(\frac{\theta_e^2 bA}{2K}\right)^{1/2} z\right] \tag{20}$$

Integrating this between $z=0$ and $z=\infty$, gives the energy of the chevron cusp for one 'arm' of the chevron:

$$E(\theta_e) = \frac{2}{3}\left(\frac{bK}{2A}\right)^{1/2} \theta_e^3 . \tag{21}$$

The total energy of the tilted layer structure is then going to be twice that given by equation (21) due to the two surfaces, and the total energy of the chevron structure will then be four times that given by equation (21), due to the additional energy cost of the cusp.

Substituting our chosen typical values for the parameters in equation (21) will allow us to estimate the energy of the various different structures. We again use $K \sim 10^{-11}$ N, and $b \sim 4.1 \times 10^4$ N m$^{-2}$ and $\theta_e \sim 0.05$ rad. Then we can estimate the energy of the tilted layer structure as being $E \sim 0.01132^{-6}$ N m$^{-1}$, while that of the chevron is $E \sim 0.02264 \times 10^{-6}$ N m$^{-1}$, leading to a difference $\Delta E \sim 0.01132^{-6}$ N m$^{-1}$. These compare well with the numerical values given above.

While giving us an idea about the energies involved, the above analysis give us insufficient information to determine the stability or otherwise of the chevron structure. This is because we have not said anything as yet about the mechanism by which a chevron structure may change into a tilted bookshelf, i.e. we have treated the total layer displacement as a constraint when solving the problem.



## 5. Surface positional anchoring

It is clear from the preceding discussion that layer positional energy would significantly alter the behaviour of the system, including which structures form the ground state at different temperatures and whether transitions between the two types of structure (tilted layers and chevrons) take place and under what circumstances. It is also evident that if there is no positional layer pinning energy, then tilted layers will be the most commonly occurring structure since they are energetically favourable. For $\theta_e < \theta_e^{tilt}$, we have a bookshelf structure, but as $\theta_e > \theta_e^{tilt}$, a transition always occurs to the tilted layer structure as there is no barrier to its formation, as can be seen from the dashed line in figure 2(*b*). Once this structure forms, it remains, with the layer tilt increasing monotonically as $\theta_e$ increases, because the tilted structure is always of lower energy than other structures.

The surface pinning forces have been investigated by Cagnon and Durand [3]. They conducted an experimental study in which a shear was applied to a liquid crystal material in the SmA phase. This was done by applying a tangential stress to one of the plates of a liquid crystal cell. The resulting lateral movement of one of the cell surfaces was recorded, and used to reconstruct the forces driving it. They observed a transmitted shear stress that had a periodic component, with the periodicity equal to the thickness of the smectic layering. This led them to conclude that the observed effects were due to surface *melting* of the smectic layering, and they measured the corresponding smectic positional anchoring energy as being $\sim 10^{-9}$ N m$^{-1}$.

Although the study of the melting process carried out by Cagnon and Durand has been extended by Elston and Towler to show that the melting of the smectic order layering order parameter under shear stress can be a complex process [8], for the purposes of the analysis presented here, we will employ a simple approximation based on the Cagnon and Durand result. We assume that the smectic layer slip takes place through a periodic near-surface melting of the smectic layering. This can be expressed as a periodic smectic layer positional anchoring energy, which we take to be:

$$E_{pos} = E^{max} \sin^2\left(\pi \frac{\Delta}{d_s}\right) \tag{22}$$

where $E^{max} \sim 10^{-9}$ N m$^{-1}$ (as measured by Cagnon and Durand), $\Delta$ represents the smectic layer displacement, and $d_s$ is the smectic layer thickness (typically $d_s \sim 2.5$ nm).

This energy will exist in addition to that already shown to be associated with the displacement of the chevron cusp from the centrosymmetric position that occurs when a tilted layer is being formed from an existing chevron. For example, adding the energy contribution due to equation (22) to the energy–displacement functions that we have already investigated, gives us an energy curve similar to that shown in figure 5.

We have seen that the uniform untilted structure is the stable, lowest energy solution for $\theta_e < \theta_e^{tilt}$. Now, however, consideration of the energies shown using the continuous lines in figure 2(*a*) and 2(*b*) (which include the effect of the layer positional energy due to surface interactions) shows that the net zero displacement structure becomes trapped in the minimum there. This means that for the regime, $\theta_e^{tilt} < \theta_e < \theta_e^{chev}$, the bookshelf structure is stabilized by the layer positional energy. Although the tilted layer structures are at lower energy levels, the energy barrier due to the positional order at the cell surfaces prevents its formation by layer slippage. Once $\theta_e > \theta_e^{chev}$, the chevron structure forms. Once again, however, its possible transition to the tilted layer structure is blocked by the surface pinning energy, as we have seen in figure 5. Thus, the formation of a stable

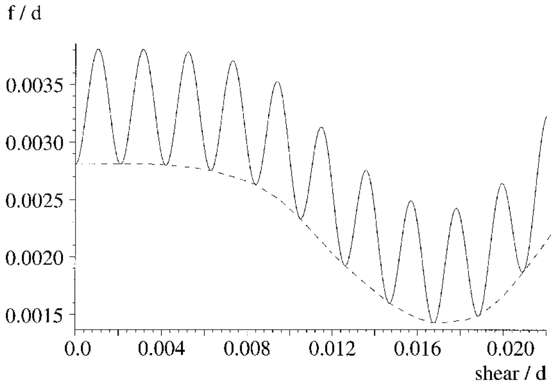


Figure 5. The effect of adding the layer positional anchoring energy to that shown in figure 3 (*c*). This is sufficient to pin the zero displacement structure, i.e. the chevron structure is stable.

chevron structure (i.e. one that does not decay or can be easily perturbed into a tilted layer structure) is shown to be critically dependent on the existence of smectic layer positional anchoring effects.

## 6. Conclusions

The features of the resulting energy curve allow us to deduce the following conclusions. Firstly, we see that structures like symmetric chevrons, which exhibit no total net layer displacement, correspond to local minima of the system, even if they are not necessarily global minima. This has been demonstrated for the $\theta_e \sim 0.025$ rad case, and is also found to be true, under the assumptions of our model, for all 'moderate' cone angles. Since the cone angle, $\theta$, is strongly coupled to the smectic layer tilt angle $\delta$ ($\theta \simeq \delta/0.85$), this also holds for all 'moderate' values of $\delta$. In figure 4 (*c*), for example, the smectic layer tilt angle $\delta \sim 0.05$ rad results in an extensive energy 'plateau' centred around zero net displacement, which means that there is little or no shearing force present at the cell surface. The energy of a periodic pinning term representing the energetics of surface melting would trap any chevron structure if it were already present (and not necessarily only symmetric chevrons). This means that the study of chevron or tilted layer formation closer to $T_{AC}$ is particularly important, since it serves to elucidate the criteria which determine which of the two structures forms and whether there is any transition between them.

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