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A model for the chevron structure obtained by cooling a smectic A liquid crystal in a cell of finite thickness

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We propose a simple model for the chevron structure observed in recent experiments by cooling a smectic A liquid crystal. We discuss the influence of the cell thickness and of the anchoring conditions on the temperature dependence of the layer tilt angle, and the formation of this structure in the vicinity of a smectic A–nematic transition. Below this critical point, a transition between a bookshelf structure and a chevron one appears. This transition is second order, with continuity of the tilt angle, the threshold being a function of the cell thickness. In addition to a classical layer thinning mechanism, we discuss another possibly based on the temperature dependence of the elastic moduli. We also propose an explanation for the existence of a critical thickness below which the chevrons do not appear.

1. Introduction

Recently, the properties of chiral smectics C in thin cells have been extensively studied [1–3] in view of the possible application of these compounds to the realization of high speed display devices. The geometry usually involved is of the bookshelf type, the layers being forced perpendicular to the cell plates by means of a suitable surface treatment. In some particular conditions, the layers become tilted, and bend in the middle plane of the cell, leading to what is called a chevron structure [2, 3]. The complete theoretical description of this structure remains to be achieved, although a simplified model built by Nagakawa [4] is now available.

In recent experiments, Takanishi *et al.* [5] and Ouchi *et al.* [6] have shown that the chevron structure was not a peculiarity of chiral smectics C, but may also be obtained by cooling a smectic A. These experiments were performed on two different liquid crystals ((4-*n*-butyloxy benzylidene-4-*n*-octylaniline) (4O.8) and 4-*n*-octyl-4′-cyanobiphenyl (8CB)), starting the cooling just above the smectic A–nematic transition, in the nematic state. Just below this transition, the X-ray diffraction pattern indicated that a bookshelf structure was formed. Upon decreasing the temperature, a chevron structure appeared, the layer tilt angle θ varying continuously from 0 to some degrees for a cooling of order 10 K. These authors suggested that this phenomenon could be due to a layer thinning effect, the temperature dependence of the layer thickness being, however, at the limit of accuracy of their detectors. The phenomenon was found to depend on the thickness of the cell, h, the main effect being a hysteresis of

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the temperature dependence of θ, for small values of h (2 and 9 μm). In addition, in the 8CB case, the chevron structure was not observed for the smallest cell thickness (2 μm) and was replaced by a uniformly tilted structure.

Here, we propose a simple model that allows us to calculate the temperature and cell thickness dependence of the tilt angle. The basic elements of this model are presented in § 2: essentially, we assume that the natural thickness a_B of the layers in the bulk of the sample is not equal to that imposed at the surface of the cell plates a_S. This may come from a temperature dependence of a_B as well as possible surface effects associated with microscopic interactions [7], and introduces a strain of the bookshelf structure $\varepsilon=(a_S-a_B)/a_B$ that should increase when the temperature is decreased. By using simple energy considerations we show that a chevron structure involving three grain boundaries such as those imagined by Bidaux *et al.* and by Kleman [8, 9], should be favoured when the strain ε applied at the boundaries becomes larger than a critical value ε_C. This threshold scales as $(h/\lambda)^2$, and $\lambda=\sqrt{(K/B)}$ being the penetration depth built on the elastic constants K and B, respectively associated with a bending and a compression of the layers. In § 3, the problem of a chevron structure in a cell of finite thickness is solved exactly. This allows us to obtain: (i) the exact value of the prefactor involved in the relationship $\varepsilon_c\approx(h/\lambda)^2$, (ii) the evolution of the chevron shape when ε is increased and in particular, (iii) the variation of the layer tilt angle as a function of both ε and h/λ. For any value of the ratio h/λ, the behaviour of $\theta(\varepsilon)$ is associated to a second order bifurcation with continuity of θ. In § 4, we discuss more precisely the influence of the temperature on θ for different experimental conditions. We show that in the case of the experiments by Ouchi *et al.*, the variation of the layer thickness (layer thinning effect) should not be the only relevant mechanism. The variation of λ with temperature in the vicinity of the smectic A–nematic transition should also influence that of θ. In particular, a mechanism of chevron formation can also be imagined based on the variation of λ even in the case of a constant mismatch ε. We also show that these considerations may perhaps explain the existence of a critical thickness below which the chevron structure does not appear and is replaced by a uniformly tilted structure. In § 5 we discuss the influence of a finite anchoring energy. All of the calculations presented in §§ 2 to 4 were based on the assumption of rigid boundary conditions, i.e. of an infinite anchoring energy. We show that these results still hold even for soft boundary conditions, the corrections being negligible in the usual experimental conditions. Finally, in § 6 we discuss the limits of our model and its possible improvements.

2. Model—simplified approach

As suggested in figure 1, we consider a cell of thickness h, containing a smectic A. At the boundaries ($x=0, h$), we assume that the layers remain always perpendicular to the solid surfaces. Practically, conditions of this kind are achieved by means of a suitable surface treatment (rubbing method after coating with PVA for instance in [5] and [6]). A small pretilt of the layers is, however, usually involved but will be neglected in the present paper. In addition to this first boundary condition, we assume that the thickness of the layers $a(x)$ is imposed in the vicinity of these surfaces ($a(x)=a_S$ at $x=0, h$), where it may differ from the natural thickness in the bulk called a_B. Two different physical origins for this situation can be imagined:

(1) As suggested by Ouchi *et al.* [6] a_B can depend weakly on temperature. If cooling is started at $T=T_0$ from an ideal bookshelf structure, with $a(x)=a_B(T_0)=a_B^0$ everywhere, a no slip condition at the boundary (or the conservation of the number

of layers in a confined geometry), can impose $a_S = a_B^0$ during the cooling process, while $a_B(T)$ is varying. If we assume a simple dependence of the kind $a_B(T) = a_B^0 (1 - \alpha\Delta T)$, where $\Delta T = T_0 - T$ is the temperature shift, the bookshelf structure suggested in figure 1 (*a*) is submitted to a strain given by

$$\varepsilon = (a_S - a_B)/a_B \approx \alpha\Delta T. \tag{1}$$

(2) Another possibility is that, because of molecular interactions, the behaviour of the layer thickness may be somewhat different at the surface of the plates from that in the bulk of the sample. This hypothesis is supported by recent observations of a crystalline order in a smectic A, frozen in the vicinity of a solid surface [7]. In this case, a_S and a_B can have their own temperature dependence. In the simplest situation, we can admit that a_S is a constant imposed by the nature of the solid. Expression (1) is then replaced by:

$$\varepsilon \approx (a_S - a_B^0)/a_B^0 + \alpha\Delta T. \tag{2}$$

In both cases, cooling the bookshelf structure will be associated with an increase of elastic energy of the cell per unit surface, the expression of which being given by

$$F_1 = \tfrac{1}{2} B h \varepsilon^2, \tag{3}$$

where B is the elastic modulus associated with a compression of the layers. Another equilibrium state of the smectic can be imagined by allowing local rotations of the layers. In a rotation of the layers through an angle $\theta(x)$, the conservation of the number of layers versus x implies that $a = a_S \cos\theta \approx a_S(1 - \theta^2/2)$. The elastic energy per unit surface is now given by

$$F = \int \left[\frac{1}{2} K \left(\frac{d\theta}{dx} \right)^2 + \frac{1}{2} B \left(\varepsilon - \frac{\theta^2}{2} \right)^2 \right] \mathrm{d}x, \tag{4}$$

where K is the elastic modulus associated with a bending of the layers, and ε is still defined as $\varepsilon(T) = (a_S - a_B)/a_B$. The minimization of F with a state of strain vanishing at infinity is a well-known problem [8, 9], whose solution is

$$\theta = \theta_\infty \tanh\left[\frac{(x - x_0)\theta_\infty}{2\lambda} \right], \tag{5}$$

with $\lambda = \sqrt{(K/B)}$ and $\theta_\infty = \sqrt{(2\varepsilon)}$. As suggested in figure 1 (*b*), a new equilibrium state compatible with the boundary conditions can be obtained by combining three grain-boundaries located at $x_0 = 0, h/2, h$. These walls, of thickness λ/θ_∞ define the frontiers of two regions where the tilt compensates the layer thinning. For this model of a chevron structure, the layer tilt angle of the chevron, and the elastic energy per unit surface of the cell are

$$\theta_\infty = \sqrt{(2\varepsilon)}, \tag{6a}$$

$$F_2 = \frac{4}{3} \sqrt{(KB)} \varepsilon^{3/2}. \tag{6b}$$

By comparing equations (3) and (6 *b*), we obtain that the chevron structure becomes the most stable configuration for ε larger than a critical value ε_c that scales as $\varepsilon_c = n(\lambda/h)^2$, n being a numerical factor (of order 7·1 in this simple approach). This effect is equivalent to the undulation instability that would occur if the layers were parallel to the cell walls [10, 11]. The dependence of ε_c upon the ratio of the two scales h and λ can

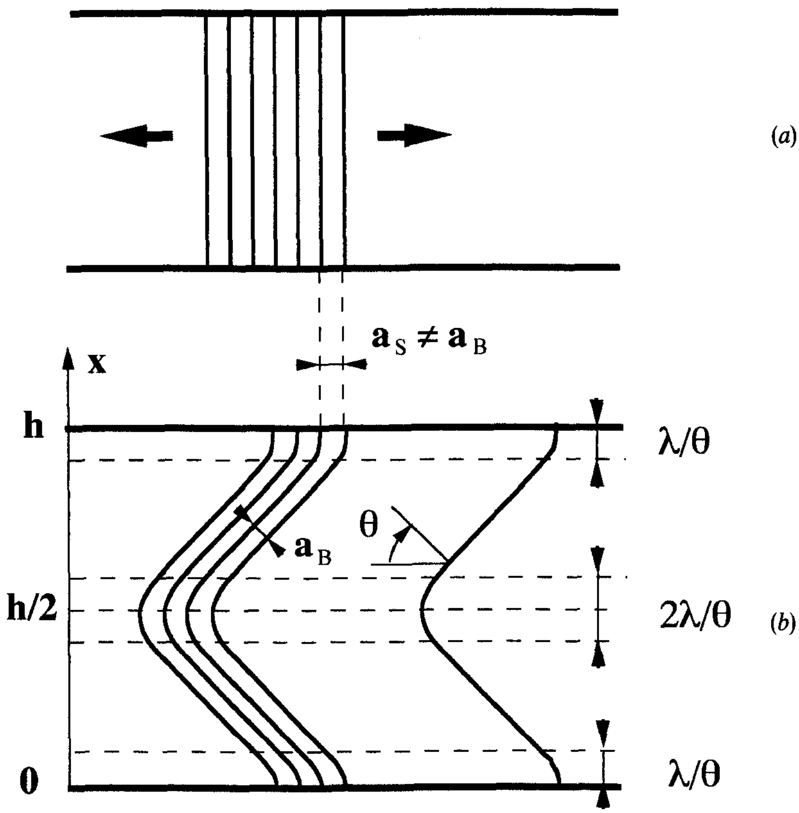

Figure 1. Upon cooling a bookshelf structure in which the layer thickness a_S is imposed at the boundaries, two different states can be imagined: (a) a bookshelf structure under mechanical tension, associated with a uniform strain $\varepsilon = (a_S - a_B)/a_B$ (a_B being the natural thickness in the bulk), and (b) a chevron structure involving three walls where the elastic energy is localized.

also be understood as follows: in the chevron structure the strain is localized in regions of thickness λ/θ, while in the bookshelf case, these regions cover in fact the whole cell of thickness h, the local strain remaining of the same order of magnitude.

We can now imagine two basic processes leading to a bookshelf–chevron transition on cooling:

(1) If we are far from the smectic A–nematic transition λ does not depend on temperature and is of the order of a few layer thicknesses. On cooling an ideal bookshelf structure, this structure will remain stable provided $\varepsilon = \alpha\Delta T$ (or $\varepsilon = \varepsilon_0 + \alpha\Delta T$) remains smaller than $\varepsilon_c \sim (\lambda/h)^2$. The chevron structure will appear just above this threshold.

(2) If the cooling is started from the smectic A–nematic transition $T_0 = T_{S_AN}$, and because of the divergence of K/B in the vicinity of this critical point, λ (and thus ε_c) should be a decreasing function of ΔT. Even in the case of a constant strain ε_0 imposed by the boundaries ($\alpha = 0$), a bookshelf–chevron transition will occur by variation of λ. In general, both effects should be involved, $\varepsilon(T)$ being an increasing function of ΔT, and $\varepsilon_c(T)$ a decreasing one. Different particular cases will be discussed in § 4.

Clearly, this simplified model of a chevron is correct only in the limit $h \gg \lambda/\theta_\infty$. In the vicinity of the bookshelf–chevron transition, the three walls overlap. The elastic energy from equation (6 *b*) is modified and we can expect that the prefactor n involved in the expression $\varepsilon_c = n(\lambda/h)^2$ will differ appreciably from the value 7·1 calculated previously. In addition, the chevron layer tilt angle which we call θ_M will differ from $\theta_\infty = \sqrt{(2\varepsilon)}$, and should be a function of both ε and the ratio h/λ. We need therefore to solve our problem exactly for any value of the cell thickness.

3. Exact solution in a cell of finite thickness

By applying the Hamilton principle, we deduce form equation (4) that we have to solve

$$\left(\frac{d\theta}{dx}\right)^2 - \frac{1}{4\lambda^2}(2\varepsilon - \theta^2)^2 = -\frac{1}{4\lambda^2}(2\varepsilon - \theta_M^2)^2, \tag{7}$$

with the boundary conditions $\theta(0)=0$ and $\theta(h/4)=\theta_M$. The right hand part of this equation is obtained by writing that the maximum tilt angle $\theta_M = \theta_M(\varepsilon, h/\lambda)$ is presumably reached at $x = h/4$, where the bending energy vanishes. θ_M is the layer tilt angle that would be measured in an X-ray diffraction experiment. We note that the analogy between our problem and the dynamics of a particle in a potential $(\theta_T^2 - \theta^2)^2$ implies that $|\theta(x)| \langle \theta_M < \theta_\infty = \sqrt{(2\varepsilon)}$. Solving equation (7), we obtain a solution of the kind:

$$\frac{x}{2\lambda} = \frac{1}{\sqrt{(4\varepsilon - \theta_M^2)}} F(\Phi, k), \tag{8 a}$$

$F(\Phi, k)$ being the elliptic integral of the first kind [12]

$$F(\Phi, k) = \int_0^\Phi \frac{1}{\sqrt{(1 - k^2 \sin^2 \phi')}} d\phi' \tag{8 b}$$

of arguments

$$\Phi = \sin^{-1}\left(\frac{\theta}{\theta_M}\right), \quad k = \frac{\theta_M}{\sqrt{(4\varepsilon - \theta_M^2)}}. \tag{8 c}$$

The equation giving θ_M as a function of ε and h/λ, is simply obtained by writing the boundary condition $\theta(h/4) = \theta_M$:

$$\frac{h}{8\lambda} = \frac{1}{\sqrt{(4\varepsilon - \theta_M^2)}} K\left(\frac{\theta_M}{\sqrt{(4\varepsilon - \theta_M^2)}}\right), \tag{9}$$

where $K(k) = F(\pi/2, k)$ is the complete elliptic integral of the first kind. We have plotted in figure 2 the evolution of θ_M versus ε for different values of the parameter h/λ and compared this variation with the asymptotic value $\theta_T(\varepsilon)$ for an infinite thickness. The finite thickness of the cell tends to reduce the tilt angle, this effect increasing when h is reduced. We see in figure 2 that the transition is second order, with continuity of the tilt angle, the threshold being dependent upon the ratio h/λ. The exact value of this threshold can be obtained easily by noting that $K(0) = \pi/2$

$$\varepsilon_c = n\left(\frac{\lambda}{h}\right)^2 \quad \text{with} \quad n = 4\pi^2. \tag{10}$$

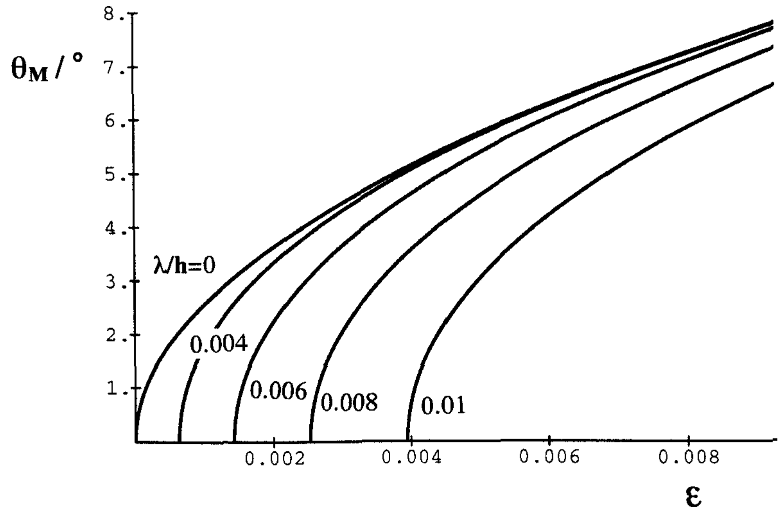

Figure 2. Dependence of the layer tilt angle on the imposed strain ε, for different values of the ratio $\lambda/h(\lambda/h=0, 0{\cdot}004, 0{\cdot}006, 0{\cdot}008, 0{\cdot}01)$.

The rather large value of the prefactor is to be noted. The simplified approach of § 1 leads to a smaller value (7·1 instead of 39·5). As we have mentioned, θ_M is a function of both ε and h/λ, and thus of both ε and $\varepsilon_c=4\pi^2(\lambda/h)^2$. When ε is close to ε_C, θ_M follows a typical mean field law, namely

$$\theta_M \approx \frac{2^{3/2}}{\sqrt{3}}\sqrt{(\varepsilon-\varepsilon_c)}. \qquad (11\,a)$$

With respect to the dependence on ε, and in the vicinity of the threshold, the influence of a variation of h reduces to a simple shift of ε_c, without modification of the function $\theta(\varepsilon-\varepsilon_c)$. Far from ε_c, θ_M tends asymptotically towards $\theta_\infty=\sqrt{(2\varepsilon)}$, the cross-over regime being given by

$$\theta_M \approx \theta_\infty\left[1-4\exp\left(-\frac{h\theta_\infty}{4\lambda}\right)\right]. \qquad (11\,b)$$

The exponential correction takes into account the overlap of the three soliton kind solutions introduced in § 2. As observed in figure 2, all of the curves tend to collapse on the curve $\theta_\infty(\varepsilon)$ for ε large enough to satisfy $\lambda/\theta_\infty \ll h$.

The dependence of θ_M on the ratio h/λ, is indicated in figure 3 for different values of ε. Just as for figure 3, two different regions described by equations (11 *a*) and (11 *b*) can be distinguished. We note again that even for a constant layer thickness ($\alpha=0$), a second order bookshelf–chevron transition can occur by cooling if λ depends on temperature, provided that ε is initially non-zero. The function $\theta_M(\Delta T)$ is to be deduced from the variation indicated in figure 3 and from the function $\lambda(T)$. This mechanism mentioned in § 2 will be discussed in more detail in the next section.

It is possible to calculate explicitly the variation of the chevron shape on ε. For a given value of k, equation (6) and (7) can be inverted to give

$$\theta(x)=\theta_M \,\mathrm{sn}\left[\frac{x\theta_M}{2\lambda k}\right], \qquad (12)$$

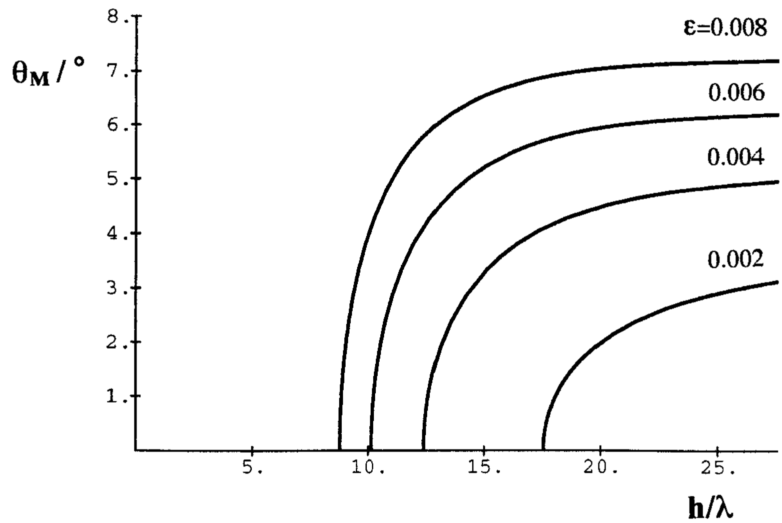

Figure 3. Dependence of the layer tilt angle on the ratio h/λ, for different values of the imposed strain $\varepsilon(\varepsilon = 0{\cdot}002, 0{\cdot}004, 0{\cdot}006, 0{\cdot}008)$.

sn being the jacobian elliptic function sn [12]. The angle $\theta(x)$ is related to the layer displacement in the y direction $u(x)$ by the relationship $\theta = \partial u/\partial x$. A simple integration gives

$$u(x) = 2\lambda\left\{\cosh^{-1}[k'] - \cosh^{-1}\left[k'\,\mathrm{dn}\left(\frac{x\theta_M}{2\lambda k}\right)\right]\right\}, \tag{13}$$

with $k' = \surd(1-k^2)$ and where we have used the jacobian elliptic function dn. Near the threshold, it is easy to check that u and θ reduce to circular functions

$$\theta(x) \approx \theta_M \sin\left(2\pi\frac{x}{h}\right), \quad u(x) \approx \frac{h\theta_M}{2\pi}\left[1 - \cos\left(2\pi\frac{x}{h}\right)\right] \tag{14}$$

that corresponds to the fundamental undulation mode of the layers in a confined geometry. Progressively this shape evolves towards the ideal chevron shape suggested in figure 1. The approximate solutions from equation (14) can also be used directly to calculate the threshold ε_c in a variational approach. Near the threshold θ^2 is small compared to ε, and the strain energy can be developed as

$$F = \tfrac{1}{2}Bh\varepsilon^2 - \tfrac{1}{2}Bh\left[\varepsilon\langle\theta^2\rangle - \lambda^2\left\langle\left(\frac{d\theta}{dx}\right)^2\right\rangle\right] + \dots \tag{15}$$

Assuming now that θ is of the kind $\theta(x) = \theta_0 \sin[2\pi(x/h)]$, we find

$$F = \tfrac{1}{2}Bh\varepsilon^2 - \tfrac{1}{4}Bh\theta_0^2\left(\varepsilon - 4\pi^2\frac{\lambda^2}{h^2}\right) + \dots \tag{16}$$

and recover the exact value of the threshold $\varepsilon_c = 4\pi^2(\lambda^2/h^2)$.

4. Different mechanisms of chevron formation: temperature dependence

We now discuss different behaviours that can be observed in the cooling of a cell of finite thickness. These different cases are indicated in figure 4.

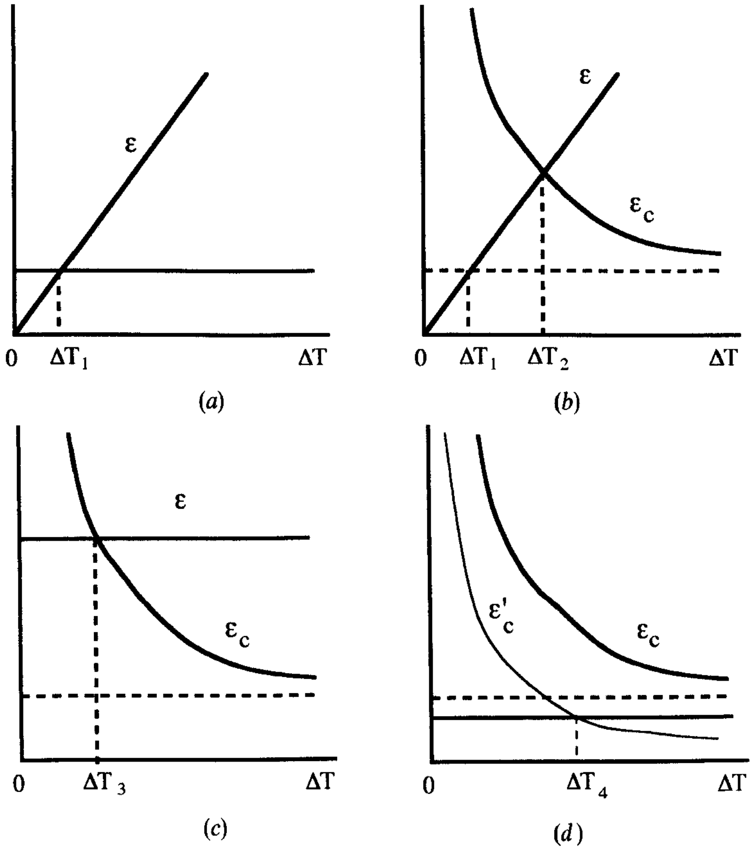

Figure 4. When cooling starts, ε grows while $\varepsilon_c \sim \lambda^{-2}$ decreases. When the two curves cross, the chevron structure appears. Different cases are suggested: (*a*) cooling far from the smectic A–nematic transition λ and thus ε_c is nearly constant; (*b*) cooling starting from the smectic A–nematic transition, because of the divergence of the bending modulus, the chevrons appear for a ΔT larger than in case (*a*); (*c*) a bookshelf–chevron transition occurs even though the layer thickness mismatch is essentially temperature independent; (*d*) same as (*c*) but for very thin cells: the chevrons never appear, but the threshold associated with a half-chevron uniformly tilted structure (curve ε_c') may be reached.

4.1. *Cooling of a smectic A far from the smectic A–nematic transition*

In the simplest case, we can imagine an experiment in which a pure bookshelf structure initially unstrained is progressively cooled, the temperature remaining very different from the critical temperature of the smectic A–nematic transition (and of any other transition temperature). As mentioned in section 1, the thermal strain reduces to $\varepsilon = \alpha\Delta T = \alpha(T_0 - T)$ and the length scale λ can be considered as a constant λ_1, usually of the order of a few layer thicknesses. In this case see figure 4 (*a*), the bookshelf structure remains stable at the beginning of the cooling ($\varepsilon < \varepsilon_c$), and is replaced by a chevron structure ($\varepsilon > \varepsilon_c$) at a critical temperature $T_1 = T_0 - \Delta T_1$ given by

$$\alpha(T_0 - T_1) = \varepsilon_c^{(1)} = 4\pi^2 \left(\frac{\lambda_1}{h}\right)^2. \tag{17}$$

The position of the threshold T_1 is difficult to estimate under the usual experimental conditions, because there are very few data concerning the temperature dependence of the layer thickness. The only data available are those of Ouchi *et al.* for 8CB that are consistent with the orders of magnitude $a_B^0 \approx 30{\cdot}5$ Å and $\alpha \approx 10^{-3}\,\mathrm{K}^{-1}$. If we assume $\lambda_1 \approx a_B^0$, we obtain a critical cooling $T_0 - T_1$ of the order 5×10^{-4} K, 5×10^{-3} K and 0·1 K for cells of thickness $h = 25\,\mu$m, 9 μm and 2 μm respectively, such as in the experiments of [6]. In this case, the effect of the cell thickness should be negligible for a cooling of a few degrees, and the approximate $\theta_M \approx \theta_\infty = \sqrt{(2\alpha\Delta T)}$ can be used. For a cooling of order 2 K, this estimate gives a layer tilt angle of order 3·5°. This value is consistent with the data obtained by Takanishi *et al.* [5], and by Ouchi *et al.* [6], which seems to support the mechanism of layer thinning that they have suggested.

In summary, the considerations developed in this section allows us to obtain good orders of magnitude for the layer tilt angle, but not for the influence of the cell thickness, measured in our simplified model by the shift of the threshold. We suggest that this may be due to the following reasons: the experiments were in fact performed starting from the nematic state. In this case, just below the smectic A–nematic transition (see the next section), the elastic modulus B depends strongly on temperature, the length scale λ being much larger than λ_1. We must now reconsider the problem of chevron formation in the vicinity of a critical point.

4.2. *Cooling in the vicinity of the smectic A–nematic transition*

In the vicinity of the smectic A–nematic transition, λ depends [13] on temperature as:

$$\lambda \approx \lambda_2 \left[\frac{T^* - T}{T^*}\right]^{-m}, \tag{18}$$

where T^* is the critical temperature of this phase transition. Usually, λ_2 is of the order of the layer thickness, and m is a critical exponent ($m \approx 0{\cdot}2$ in most cases). From equation (10), we deduce that the chevron structure will appear if

$$\varepsilon(T) > \varepsilon_c^{(2)}(T) = 4\pi^2\left(\frac{\lambda_2}{h}\right)^2\left[\frac{T^* - T}{T^*}\right]^{-2m}, \tag{19 a}$$

with

$$\varepsilon(T) = (a_S - a_B)/a_B = (a_S - a_B^*)/a_B^* + \alpha(T^* - T), \tag{19 b}$$

where in analogy with section 2, we have designated by a_B^* the natural thickness of the layer at the smectic A–nematic transition and by a_S the thickness imposed at the boundaries. For simplicity, we only discuss the case $a_S = a_B^*$ in this section, the influence of an initial strain being treated in the next one. As observed in figure 4 (*b*), the evolution observed in the cooling process is not modified qualitatively: just below T^*, a bookshelf structure appears, and breaks into a chevron one at a critical temperature T_2 given by:

$$\alpha(T^* - T_2) = [4\pi^2(\lambda_2/h)^2]^{1/(1+2m)}[\alpha T^*]^{2m/(1+2m)}. \tag{20}$$

For 8CB, $T^* = 306{\cdot}5$ K, and $m \approx 0{\cdot}2$ together with $\lambda_2 \approx a_B^* \approx 30{\cdot}5$ Å lead to values of order $T^* - T_2 \approx 0{\cdot}02$ K, 0·1 K and 1 K, respectively for the studied cell thicknesses $h = 25\,\mu$m, 9 μm and 2 μm. The effect of the cell thickness is now not negligible in a cooling of a few degrees. The quantity $T^* - T_2$ is larger than $T^* - T_1$ because λ can be much larger than λ_1 near T^*, and depends on h as $h^{-1/(1+2m)}$($h^{-0{\cdot}7}$ for $m = 0{\cdot}2$) instead of h^{-2}. We have plotted in figure 5 the typical variation of θ_M versus T for different values of the ratio λ_2/h. This variation combines now both dependences of θ_M upon ε and h/λ depicted in figures 2 and 3. The behaviour obtained is however very similar to

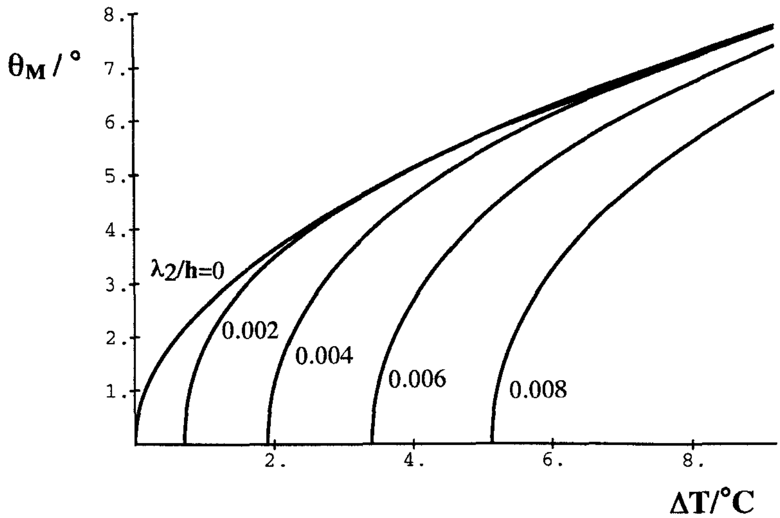

Figure 5. In the case of figure 4 (*b*) ($\varepsilon(T^*)=0$, see § 4,2), evolution versus $\Delta T=T^*-T$ of the layer tilt angle for $\lambda_2/h=0, 0{\cdot}002, 0{\cdot}004, 0{\cdot}006, 0{\cdot}008$.

that of figure 2. We again have a bifurcation associated with a second order transition, that can also be described near T_{BC} by equation (10). By combining equations (11 *a*), (18) and (20), it is possible to pin down the behaviour of θ_M near the bifurcation

$$\theta_M \approx \frac{2^{3/2}}{\sqrt{3}} \sqrt{[\alpha(1+2m)(T_{BC}-T)]}. \tag{21}$$

Far from T_{BC}, θ_M tends to the asymptotic value $\theta_T=[2\alpha(T^*-T)]^{1/2}$ associated with an infinite thickness.

In summary, when the divergence of λ is taken into account the influence of the cell thickness may become measurable. In our model, this effect reduces to a shift of the threshold that scales as $h^{2/(1+2m)}$, m being the exponent of the length λ.

4.3. *Cooling near the smectic A–nematic transition with an initial tension*

We still consider the case of a cooling started in the nematic state, but we now assume that a_S is larger than a_B^*. As the growth of the layers presumably begins near the solid surfaces, the thickness $a_B=a_S$ will be imposed in the bulk and the bookshelf structure formed at T^* should be under tension: $\varepsilon(T^*)=(a_S-a_B^*)/a_B^* \neq 0$.

For simplicity, we admit that the temperature dependence of a_S and a_B can be neglected: ε remains constant while ε_c depends on temperature. As indicated in figure 4 (*c*), a bookshelf–chevron transition also occurs in this case by variation of λ. The position of the threshold is obtained by writing that $\varepsilon=\varepsilon_c$, which gives

$$\frac{T^*-T_3}{T^*} \approx \left[4\pi^2\left(\frac{\lambda_0}{h}\right)^2 \frac{1}{\varepsilon(T^*)}\right]^{1/2m}. \tag{22}$$

Now, T^*-T_3 scales as $h^{-1/m}$ ($\approx h^{-5}$ for $m=0{\cdot}2$). Below T_3, the behaviour of θ_M is to be deduced from its dependence on h/λ indicated in figure 3. The main difference with the other cases is that θ_M should saturate at the value $\theta_\infty \approx \sqrt{[2\varepsilon(T^*)]}$ for large values of T^*-T. Concerning the orders of magnitude, an initial strain of order $0{\cdot}01$ ($\theta_\infty \approx 10°$) with the estimate $\lambda_2 \approx a_B^* \approx 30\cdot5$ Å leads to $T^* - T_3 \approx 0\cdot06$ K in a cell of $2\,\mu$m of 8CB. This value is rather small, but depends strongly on the prefactor of λ_2. For instance, an estimate based on $\lambda_2 \approx 3a_B^*$ is somewhat higher: $T^* - T_3 \approx 2$ K.

The main interest of this mechanism of chevron formation is that it may explain the observation of a critical thickness h^* below which the chevron structure does not appear. Far from T^*, we may expect that $\lambda(T)$ should tend to the value λ_1 introduced in § 4.1. As indicated in figure 4 (d), $\varepsilon_c(T)$ should tend to the associated value $\varepsilon_c^{(1)} = 4\pi^2\lambda_1^2/h^2$ and should remain bounded from below. If at the smectic A–nematic transition $\varepsilon(T^*)$ is smaller than $\varepsilon_c^{(1)}$, the chevron structure will never appear. The critical thickness is thus defined by the equality $\varepsilon(T^*) = \varepsilon_c^{(1)}$ which gives

$$h^* = 2\pi \frac{\lambda_1}{\sqrt{[\varepsilon(T^*)]}}, \tag{23}$$

with the same orders of magnitude as previously, $\lambda_1 \approx a_B \approx 30\cdot5$ Å and $\varepsilon(T^*) \approx 0\cdot01$, we find $h^* \approx 0\cdot2\,\mu$m. This value is ten times smaller than the experimental value obtained by Ouchi *et al.* for 8CB.

In addition to the strained bookshelf structure, we can imagine the possibility of a uniformly tilted structure involving only two walls, such as those of figure 1. In other words, this would correspond to a half-chevron structure, deduced from the chevron associated with a thickness $2h$. As indicated in figure 4 (d), the threshold ε_c becomes four times smaller than for the complete chevron structure, and a range of temperature appears where the half-chevron structure is possible, but not the chevron one. This is precisely reminiscent of the observations of Ouchi *et al.*, who found that for small enough cells, only the uniformly tilted structure was stable. We still have to understand how this uniformly tilted structure can be formed.

5. Influence of the anchoring energy

All of the calculations presented in the previous sections were based on the assumption of rigid boundary conditions: $\theta(x) = 0$ for $x = 0$ and h. More realistic conditions are obtained by assuming a finite anchoring energy W, the total energy being

$$F = \int_0^h \left[\frac{1}{2}K\left(\frac{d\theta}{dx}\right)^2 + \frac{1}{2}B\left(\varepsilon - \frac{\theta^2}{2}\right)^2\right] dx + W[\theta^2(x=0) + \theta^2(x=h)]. \tag{24}$$

The bulk equation (7) still holds, but the boundary conditions are now of the kind $e(d\theta/dx) = \pm\theta, e = K/W$ being a typical anchoring length [11]. We have now to evaluate the influence of this finite value W on the threshold value ε_c.

In the simplest approach, we can say that the new value of the threshold ε_{c2} will remain bounded between the values associated with the rigid and soft cases: $W = \infty$ and $W = 0$. The soft case value can easily be deduced from the approximate form of the bulk energy [16], the fundamental mode being now of wavelength $2h$ instead of h: $\theta(x) \approx \theta_0 \cos[\pi(x/h)]$. The value obtained coincides with the threshold that would be obtained in a cell of thickness $2h$ with rigid conditions: $\varepsilon_{c2} = \pi(\lambda^2/h^2)$. We obtain then that the threshold will remain bounded: $\pi(\lambda^2/h^2) < \varepsilon_c < 4\pi(\lambda^2/h^2)$. This suggests that the different scenarios of chevron formation suggested in § 4 will not be significantly affected and will still roughly hold with a slight modification of the orders of magnitude. In fact, as we will see, the correction to the rigid case is very small under the usual experimental conditions.

To be more precise, we have to assume that, in the vicinity of the threshold, $\theta(x)$ is a combination of the two limiting cases

$$\theta(x) \approx \theta_1 \cos\left(\pi \frac{x}{h}\right) + \theta_2 \cos\left(2\pi \frac{x}{h}\right). \tag{25}$$

A number that measures the influence of W(or of the scale $e = K/W$) on the difference $4\pi(\lambda^2/h^2) - \varepsilon_c$ can be built very easily as the ratio of the order of magnitude of the surface energy $F_S = (K/e)\theta_1^2$ to that of the bulk energy $F_B = (K/h)\theta^2$

$$\beta = \frac{F_S}{F_B} = \frac{e}{h}. \tag{26}$$

When this parameter is small, ε_c remains close to the rigid case. The correction can be calculated by using the variational approach discussed at the end of § 3, the test function being now of the kind from equation (25). This finally gives an approximate energy

$$F \approx \tfrac{1}{2} Bh\varepsilon^2 - B\frac{h}{2} Q(\theta_1, \theta_2) + \dots$$

with

$$Q(\theta_1, \theta_2) = \frac{1}{2}\left(\varepsilon - \pi^2 \frac{\lambda^2}{h^2} - 4\frac{e}{h}\right)\theta_1^2 + \frac{1}{2}\left(\varepsilon - 4\pi^2 \frac{\lambda^2}{h^2}\right)\theta_2^2 + \frac{8}{3\pi}\left(\varepsilon - \pi^2 \frac{\lambda^2}{h^2}\right)\theta_1\theta_2. \tag{27}$$

The threshold is reached when one of the eigenvalues vanishes, which leads to

$$\left(\varepsilon_c - \pi^2 \frac{\lambda^2}{h^2}\right)\left(\varepsilon_c - 4\pi^2 \frac{\lambda^2}{h^2}\right) = \frac{64}{9\pi^2}\left(\varepsilon_c - \pi^2 \frac{\lambda^2}{h^2}\right)^2. \tag{28}$$

In the limit of small α, the relevant solution of this equation reduces to

$$\varepsilon_c = 4\pi \frac{\lambda^2}{h^2}[1 - 4\beta + \dots]. \tag{29}$$

Usually, for clean surfaces e is of a molecular size and weakly temperature dependent. In this case, corrections involved in equation (29) are negligible and rigid boundary conditions prevail.

6. Discussion—possible improvements

In summary, we have built a simplified model for the problem of chevron formation by cooling a smectic A. This model allows us to recover some qualitative observations of Ouchi *et al.*, and also reasonable orders of magnitude for the influence of the cell thickness: temperature dependence of the tilt angle for thick cells (with good orders of magnitude), correct orders of magnitude for the cell thicknesses at which finite size modifies the results, and the possible existence of a critical thickness below which the chevrons do not appear. However various unknown parameters enter this model, and some experimental observations are not explained: the existence of an hysteresis at intermediate thicknesses instead of a shift of the threshold and the formation of focal conics.

We think that the next step would involve solving the problem after allowing a slight pretilt of the layers near the solid plates. The existence of this pretilt is mentioned in the paper of Ouchi *et al.* Preliminary calculations [15] suggest that instead of being second order, the transition could be first order in this case with a discontinuity of the tilt angle. This can lead to hysteretic effects similar to those found by Ouchi *et al.* In addition, these experimental results raise a question concerning the experimental conditions: is the stationary state really reached in the time of the experiment? The hysteresis may possibly be attributed to problems of delay in the evolution towards equilbrium.

Finally, it is interesting to mention the similarity of the chevron problem with that of buckling of beams or plates [16]. Basically, we have compared an energy associated to a uniform strain with another associated to a bending phenomenon, and found just as for the buckling problem a threshold on the applied stress. From this point of view, the chevron formation with an initial pretilt of the layer of opposite value on each plate is very similar to the problem of buckling of a beam with an initial curvature. We can expect in this case, the occurrence of an imperfect bifurcation, the experimental consequences of which will be discussed in a future paper [15].

Another possible improvement of our model would be to introduce dislocations in the layers that could eventually collapse in focal conic structures. This phenomenon could be equivalent to that imagined by Williams and Kléman [17], in the theoretical treatment of thin cells of smectics A under shear. However, it should not occur at small enough mismatch parameter ε, since the energy of a dislocation wall goes linearly with ε, whereas the chevron energy goes as $\varepsilon^{3/2}$. Note that another model of the chevron based on distributions of disclinations has been proposed recently by Lejcek [14].

Finally, let us point out that experiments performed near the bookshelf–chevron threshold, and also investigations of the layer behaviour near the cell walls could greatly enlighten these attempts of modellization.

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