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# Biaxial modeling of the structure of the chevron interface in smectic liquid crystals

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We have included the inherent molecular biaxiality of the smectic $C$ phase in a model of the chevron structure. This molecular biaxiality is related to a hindered rotation about the molecular long axis which for chiral, polar molecules induces a spontaneous polarization. Through the coupling between biaxiality and the smectic cone angle, continuity of the molecular distribution at the chevron interface leads to changes in the cone angle. Under certain approximations we are able to find analytic expressions for the chevron structure and consequently estimate the width of the chevron interface. There are in fact two correlation lengths which govern variations in the cone angle and the biaxiality. [S1063-651X(99)06207-8]

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## I. INTRODUCTION

Considerable effort has been expended in recent years on the development of continuum theories for smectic $C$ ($S_C$) and chiral smectic $C$ ferroelectric liquid crystals ($S_C^*$ or FLC). This research has been partly motivated by scientific interest, but also because of the considerable potential for exploitation of ferroelectric liquid crystals in display devices. Commercial interest has largely centered on understanding the structures formed and the switching within surface-stabilized homogeneously aligned cells. One of the most characteristic structures found within these cells is the ''chevron.'' This was first observed in surface-stabilized ferroelectric liquid crystal (SSFLC) cells using x-ray diffraction, in the $S_C^*$ phase [1,2], and confirmed optically using a guided mode technique [3]. The chevron structure has subsequently been found in thicker cells [4] and in the smectic $A$ ($S_A$) phase [5]. The presence of two peaks in the diffraction trace corresponded to equal and opposite layer tilts, $\pm\delta$, with a sharp transition between them. Rieker *et al.*[2] demonstrated the independence of the layer tilt $\delta$ from the treatment of the cell surfaces, and its dependence on the cone angle $\theta$. Experimental studies have since estimated the chevron ''tip'' thickness to be $\approx 10^{-8}$ m [2]. In addition, high resolution x-ray studies have shown the existence of triple peaks within FLC cells [5]. These are taken to come about due to the presence of a double kink chevron structure [6].

The chevron structure is believed to form due to the mismatch between the prescribed $S_A$ layer thickness at the cell surfaces and the layer thickness within the bulk of the cell which is determined by the smectic cone angle $\theta$. This layer thickness matching condition can be satisfied by tilting the layers away from the cell surface normal.

Clark and Rieker put forward the original theoretical model [7] of the chevron, which explained it in terms of a *kink* or discontinuous change in the smectic layering. Although this model has a discontinuity in the layer tilt $\delta$, the $\mathbf{n}$-director structure is continuous at the chevron interface.

Since then a number of other models of the chevron interface have been put forward [8–13]. Generally, a feature that these models have in common is that the discontinuity in $\delta$ is avoided by allowing one or more of the parameters of the system such as the layer tilt $\delta$, the cone angle $\theta$, the azimuthal angle around the smectic cone $\phi$, or the layer thickness, to vary smoothly within the cell.

Nakagawa [8] proposed a continuous model based on the minimization of an energy consisting of terms from layer dilation, layer bending, and variations of $\phi$.

In [9], Limat and Prost described the chevron structure in terms of the layer tilt angle $\delta$, which was assumed to be continuous across the cell. By writing the free energy in terms of $\delta$ they were able to investigate the second order transition between the smectic $A$, bookshelf structure, and the smectic $C$, chevron structure.

By assuming that the layer tilt $\delta$ was coupled to $\theta$ and then allowing $\theta$ to vary through the cell De Meyere *et al.* [10] were able to remove the layer tilt discontinuity while preserving the layer thickness. In their model balancing energy contributions from layer curvature and variations in $\theta$ they found solutions for the chevron structure. The assumption of constant layer thickness and layer curvature leads to the necessary condition that $\theta$ is zero at the chevron interface, i.e., the liquid crystal is in the smectic $A$ phase.

Limat [11] later extended the previous model of Nakagawa to included the possibility that the layer tilt angle does not equal the smectic cone angle.

Vaupotič *et al.* [12,13] removed the constant layer thickness condition and found solutions for which $\theta$ is nonzero but small at the chevron interface where there is a small region of layer dilation.

## II. MODELING

All the models outlined in the preceding section do not include the inherent molecular biaxiality of the smectic $C$ phase. This molecular biaxiality (illustrated in Fig. 1) is related to a hindered rotation about the molecular long axis which for chiral, polar molecules induces a spontaneous polarization. Figure 1 shows the biaxial molecule, in a simplistic representation, as a rectangular cuboid with no equal side lengths. The macroscopic variable $\mathbf{a}$ is defined as the vector normal to the smectic layer while the variables $\mathbf{n}_i$, $\mathbf{m}_i$, $\theta_i$,

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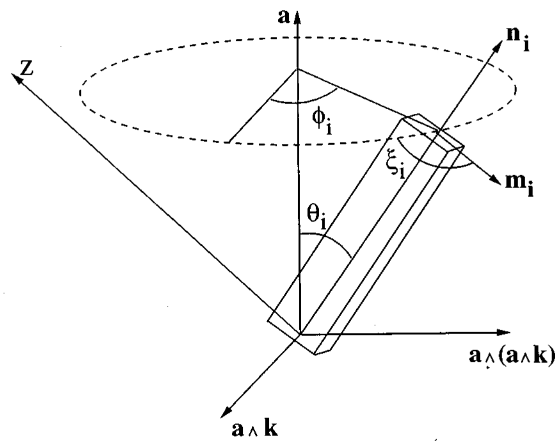

FIG. 1. Configuration of the biaxial liquid crystal molecule. The vectors **a** and **k** are parallel to the smectic layer normal and the $z$ axis, respectively. The major molecular axis $\mathbf{n}_i$ is described by the cone angle $\theta_i$ and the azimuthal angle $\phi_i$. The intermediate molecular axis $\mathbf{m}_i$ is described by the angle $\xi_i$.

$\phi_i$, and $\xi_i$ are defined for *each* molecule. In this paper we will assume that the order parameters associated with the molecular distribution of $\theta_i$ and $\phi_i$ are constant thus the macroscopic director $\mathbf{n}=\langle \mathbf{n}_i \rangle$ can be defined by the macroscopic variables **a**, $\theta=\langle \theta_i \rangle$, and $\phi=\langle \phi_i \rangle$, where $\langle\,\rangle$ denotes the average value of the variable. The vector $\mathbf{m}_i$ is in the direction of the molecular dipole of the molecule while $\xi_i$ is the angle of rotation of the molecule about the long axis. We will assume that the average value $\mathbf{m}=\langle \mathbf{m}_i \rangle$ remains constant and perpendicular to **a** and **n** (i.e., tangential to the smectic cone) while the order parameter defined by [14]

$$S=\langle \cos(2\xi_i) \rangle \tag{1}$$

is allowed to vary. This definition implies that when all molecules are perfectly aligned with **m** (i.e., $\mathbf{m}_i=\mathbf{m}$ or $\xi_i=0$ for all molecules), $S=1$, and when the molecules are randomly oriented around the molecular long axis (i.e., $\mathbf{m}_i$ or $\xi_i$ are random), $S=0$. When the molecules are all perpendicular to **m** (i.e., $\mathbf{m}_i \cdot \mathbf{m}=0$ or $\xi_i=\pm\pi/2$ for all molecules) then $S=-1$. We can now describe the smectic $C$ phase in terms of the macroscopic variables, the layer normal **a**, the *nematic-like* director **n**, and $S$ the biaxial order parameter. Figure 2 gives a pictorial representation of a chevron in a surface-stabilized FLC cell. It is assumed that the layer normal **a** lies in the $xz$ plane and thus may be described simply by the layer tilt angle $\delta$. The nematiclike director **n** is described by the cone angle $\theta$ and the azimuthal angle $\phi$. These variables will be allowed to vary along the cell normal, i.e., the $z$ direction. Figure 3 illustrates the importance of including the biaxial order parameter in our description of the chevron. If the biaxial order parameter is nonzero the molecular distribution of the biaxial molecules will be elongated either along the tangent to the cone or perpendicular to the tangent to the cone. In a FLC material this would result in the spontaneous polarization lying tangential or perpendicular to the smectic cone. Figure 3(a) shows that on either side of the chevron interface there exists a mismatch of the molecular distributions. It is obvious that such a discontinuity is rectified by insisting that the biaxial order parameter is zero at the chevron interface so that the system is uniaxial there [Fig. 3(b)]. As we will see later, since the biaxial order parameter is coupled to the smectic cone angle $\theta$ the condition that $S=0$ at the chevron implies that $\theta$ will also change in this region.

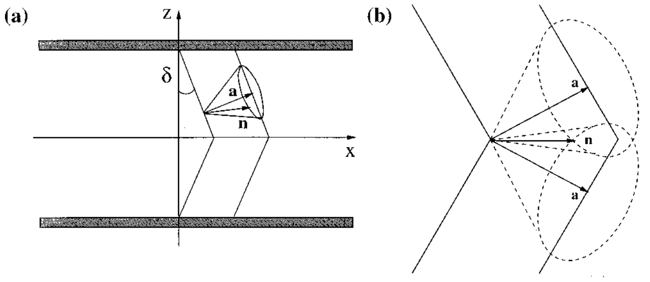

FIG. 2. The chevron configuration within the surface-stabilized FLC cell. (a) In the region $z>0$ the smectic layer is tilted by an angle $\delta$ while in the region $z<0$ the layer tilt angle is $-\delta$. The chevron interface lies at $z=0$. (b) At the chevron interface continuity of the director structure implies that **n** lies on the intersection of two smectic cones.

Although biaxial order is known to exist in SSFLC cells through the existence of a spontaneous polarization none of the presently published models of chevron structures include it. In this paper we will extend the original model of Clark and Rieker to include continuity of biaxial ordering.

We start with a simple model describing the bulk of a liquid crystal sample. The energy density $f_{\text{bulk}}$ near the phase transition $T_{AC}$ is given by the simple Landau–de Gennes expansion in terms of the cone angle $\theta$,

$$f_{\text{bulk}}=f_0+\frac{a}{2}\theta^2+\frac{b}{4}\theta^4+\frac{c}{6}\theta^6, \tag{2}$$

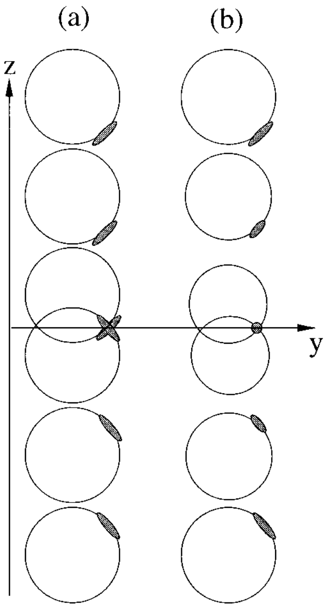

FIG. 3. (a) With a fixed value of the biaxial order parameter $S$ the molecular distributions do not coincide at the chevron interface. (b) If the biaxial order parameter is allowed to vary, $S$ is continuous at the chevron interface. Since they are intrinsically coupled, variations in $S$ are accompanied by variations in the cone angle $\theta$.

where $a=\alpha(T-T_{AC})$. We then incorporate biaxial ordering into this model by including an order parameter $S$. We can now write down an expression for the energy density describing a biaxial liquid crystal in the bulk as a function consisting of an expansion in terms of two order parameters, the cone angle $\theta$ and the biaxial measure $S$.

$$f_{\text{bulk}}=f_0+\frac{a}{2}\theta^2+\frac{b}{4}\theta^4-\frac{q}{2}S\theta^2+\frac{3}{4}AS^2, \tag{3}$$

where we have neglected the higher order terms $O(\theta^6)$, $O(S^3)$. Because of the invariance of the energy under the symmetry operation $\theta\rightarrow-\theta$ but not under $S\rightarrow-S$, the coupling between $\theta$ and $S$ is represented by the $O(S\theta^2)$ term.

In order to simplify this expression, it is useful to consider what the equilibrium values of the two parameters $\theta$ and $S$ might be for this system. These stationary points of the free energy are found by differentiating Eq. (3) with respect to $\theta$ and $S$,

$$0=a\theta+b\theta^3-qS\theta, \tag{4a}$$

$$0=-\frac{q}{2}\theta^2+\frac{3}{2}AS. \tag{4b}$$

From Eq. (4b) the equilibrium values for $\theta$ and $S$ are

$$\theta=0,\quad S=0, \tag{5a}$$

$$\theta=\theta_e,\quad S=\frac{q}{3A}\theta_e^2, \tag{5b}$$

$$\theta=-\theta_e,\quad S=\frac{q}{3A}\theta_e^2, \tag{5c}$$

where

$$\theta_e=\left(\frac{3aA}{q^2-3bA}\right)^{1/2} \tag{6}$$

is the nonzero equilibrium value of $\theta$. The nonzero equilibrium value of $S$ is then $S_e=qa/(q^2-3bA)$. Therefore, while $\theta_e$ is proportional to the square root of the temperature difference, $\Delta T=T-T_{AC}$ [from Eq. (6) with $a=\alpha(T-T_{AC})$], $S_e$ grows linearly with $\Delta T$. From Eq. (6) $\theta_e$ is imaginary in the smectic $A$ phase. Solution (5a) therefore corresponds to the smectic $A$ phase and solutions (5b) and (5c) correspond to smectic $C$ phases with opposite tilt angles. These solutions are stable if

$$\frac{d^2F}{dS^2}>0, \tag{7a}$$

$$\frac{d^2F}{d\theta^2}>0, \tag{7b}$$

$$\left(\frac{d^2F}{dS^2}\right)\left(\frac{d^2F}{d\theta^2}\right)-\left(\frac{d^2F}{dSd\theta}\right)^2>0. \tag{7c}$$

For the smectic $A$ phase ($\theta=0$, $S=0$), these conditions imply $A>0$, $a>0$ and for the smectic $C$, tilted, phase ($\theta=\pm\theta_e$, $S=S_e$) they imply $A>0$, $a<0$, $b>0$, $q^2-3bA<0$. The conditions $A>0$ and $b>0$ are in fact necessary in order to be able to write a Landau expansion (3) for the smectic $C$ phase. The conditions $a>0$ and $a<0$ are clearly equivalent to $T>T_{AC}$ and $T<T_{AC}$ as expected. The condition $q^2-3bA<0$ for the smectic $C$ phase to exist is more subtle. The $b$ and $A$ terms in the Landau expansion (3) tend to reduce the cone angle and biaxial order parameter while the $q$ term tends to increase both $\theta$ and $S$. In order for the smectic $C$ phase to exist these three terms must reach a balance such that $\theta$ and $S$ are nonzero and finite. If, however, $q$ is too large, the free energy has no minimum for *any* values of the cone angle and the biaxiality. The bound on $q$ is given by the condition $q^2<3bA$.

Using the above expressions for $\theta_e$ and $S_e$ we can rearrange the free energy density (3) into

$$f_{\text{bulk}}=f_0'+\frac{b}{4}\left[\theta^2-\theta_e^2\left(1-\frac{3AS_e^2}{b\theta_e^4}\right)\right]^2+\frac{3}{4}AS\left(S-\frac{2S_e\theta^2}{\theta_e^2}\right), \tag{8}$$

which is independent of the parameters $a$ and $q$. In Eq. (8) $f_0'$ is a constant energy term.

Equation (8) is insufficient on its own to describe the structure of the chevron interface. To do this we need to be able to describe how the order parameters vary in the vicinity of the chevron tip.

First, we postulate that the entropic biaxiality order parameter $S$ varies smoothly in the vicinity of the chevron tip. The changes in order associated with this melting can be represented by gradient terms in $S$:

$$f_{\text{ent}}=\frac{\kappa}{2}\left(\frac{dS}{dz}\right)^2, \tag{9}$$

where $\kappa$ represents the entropic cost of gradients in the $S$ order parameter and $z$ is the coordinate in the direction of the cell normal.

In order to describe the elasticity that governs distortions in the director structure near an interface such as the chevron or a cell surface, we assume that the biaxiality plays only a minor part in any such distortion, allowing us to write a term that will describe the variation in the director **n** (across the cell thickness) by a nematiclike elastic energy,

$$f_{\text{elas}}=\frac{K}{2}[(\boldsymbol{\nabla}\cdot\mathbf{n})^2+(\boldsymbol{\nabla}\times\mathbf{n})^2], \tag{10}$$

where $K$ is an elastic constant and a one constant approximation to the elasticity has been used.

From Figs. 1 and 2 the director **n** may be written as

$$\mathbf{n}=(\cos\theta\cos\delta+\sin\theta\sin\phi\sin\delta,-\sin\theta\cos\phi,\cos\theta\sin\delta-\sin\theta\sin\phi\cos\delta). \tag{11}$$

Since all the variables $\delta$, $\theta$, and $\phi$ may depend on $z$, the elastic energy (10) is complicated. In order to make the system analytically tractable we will make certain simplifying assumptions.

For the director to be continuous at the chevron interface **n** must lie in the plane of the cell surfaces. We will assume that in a region around the interface the director stays roughly in the $xy$ plane. In terms of the relevant angles this condition is

$$\sin\phi = \frac{\tan\delta}{\tan\theta}. \tag{12}$$

Near to the interface we may also assume that the azimuthal angle is approximately constant so that $\phi = \phi_0$ (the value at $z = 0$, the chevron interface). Lastly we will assume that both the layer tilt angle $\delta$ and the cone angle $\theta$ are small. This approximation is valid in the vicinity of the smectic $A$ to $C$ phase transition (i.e., $T \approx T_{AC}$). With the above assumptions the director may then be written as

$$\mathbf{n} = (1, -\theta\cos\phi_0, 0), \tag{13}$$

and the elastic energy simplifies to

$$f_{\text{elas}} = \frac{K}{2}\cos^2\phi_0\left(\frac{d\theta}{dz}\right)^2. \tag{14}$$

We may estimate the constant azimuthal angle using the relationship (12) to write

$$\cos^2\phi_0 = 1 - \left(\frac{\tan\delta_0}{\tan\theta_0}\right)^2 \approx 1 - \left(\frac{\delta_0}{\theta_0}\right)^2. \tag{15}$$

Equations (8), (9), and (14) with (15) can now be combined and used to write an expression for the energy density of the system in the vicinity of a chevron interface:

$$f = f_0' + \frac{K'}{2}\left(\frac{d\theta}{dz}\right)^2 + \frac{b}{2}\left[\theta^2 - \theta_e^2\left(1 - \frac{3AS_e^2}{b\theta_e^4}\right)\right]^2 + \frac{\kappa}{2}\left(\frac{dS}{dz}\right)^2 + \frac{3}{4}AS\left(S - \frac{2S_e\theta^2}{\theta_e^2}\right), \tag{16}$$

where $K' = K(1 - \delta_0^2/\theta_0^2)$.

We can simplify the above free energy density with the following normalizations and nondimensionalization:

$$\Theta = \frac{\theta}{\theta_e}, \tag{17a}$$

$$\sigma = \frac{S}{S_e}, \tag{17b}$$

$$Z = z\left(\frac{3A}{2\kappa}\right)^{1/2}, \tag{17c}$$

$$\lambda = \frac{3AS_e^2}{b\theta_e^4}, \tag{17d}$$

$$\alpha = \frac{3AK'}{2b\kappa\theta_e^2}, \tag{17e}$$

$$F = \frac{4(f - f_0')}{3AS_e^2}. \tag{17f}$$

The nondimensionalized free energy density is then

$$F = \frac{2\alpha}{\lambda}\left(\frac{d\Theta}{dz}\right)^2 + \frac{1}{\lambda}[\Theta^2 - (1-\lambda)]^2 + \left(\frac{d\sigma}{dz}\right)^2 + \sigma(\sigma - 2\Theta^2). \tag{18}$$

We minimize the energy by solving the Euler-Lagrange equations of the system to find the manner in which $\Theta$ and $\sigma$ vary in the vicinity of the chevron interface. For Eq. (18) the Euler-Lagrange equations are

$$0 = \frac{d^2\sigma}{dZ^2} - \sigma + \Theta^2, \tag{19a}$$

$$0 = \alpha\frac{d^2\Theta}{dZ^2} + \Theta[1 - \Theta^2 + \lambda(\sigma - 1)]. \tag{19b}$$

Far from the chevron interface in the bulk of the liquid crystal the structure will be uniform and $d^2\Theta/dz^2 = d^2\sigma/dz^2 = 0$. Then Eqs. (19) give the solutions

$$\sigma = 0, \quad \Theta = 0, \tag{20a}$$

$$\sigma = 1, \quad \Theta = 1, \tag{20b}$$

$$\sigma = 1, \quad \Theta = -1, \tag{20c}$$

which are equivalent to the bulk solutions of Eqs. (5). It is also worthwhile noting that the stability condition for the tilted smectic $C$ phase, $q^2 - 3Ab < 0$, is equivalent to $\lambda < 1$. The other stability conditions, $A > 0$ and $b > 0$, ensure that $\lambda \geqslant 0$.

The governing equations (19) will subsequently be solved subject to certain relevant boundary conditions. If we fix the chevron interface at $z = 0$ then, as discussed above, smooth changes in the molecular distribution will only take place if the azimuthal orientational fluctuations around the long molecular director are isotropic at the interface, i.e., $S = 0$.

Far from the chevron tip, within the bulk of the liquid crystal cell, it seems reasonable to expect the cone angle and the biaxial order parameter to be equal to their equilibrium values, that is, $\theta = \pm\theta_e$ and $S = S_e$. In terms of nondimensionalized variables, this corresponds to the condition $\Theta = \pm 1$ and $\sigma = 1$. The full boundary conditions are thus

$$\Theta \to \pm 1 \quad \text{as } Z \to \pm\infty, \tag{21a}$$

$$\sigma \to 1 \quad \text{as } Z \to \pm\infty, \tag{21b}$$

$$\sigma = 0 \quad \text{at } Z = 0. \tag{21c}$$

The first boundary condition (21a) leads to two distinct possibilities for the director structure at $z = 0$. If $\Theta \to +1$ as $z \to +\infty$ and $\Theta \to -1$ as $z \to -\infty$ (or equivalently $\Theta \to -1$ as $z \to +\infty$ and $\Theta \to +1$ as $z \to -\infty$) continuity of the director structure implies that $\Theta = 0$ at $z = 0$. However, $\Theta \to +1$ as $z \to +\infty$ and $\Theta \to +1$ as $z \to -\infty$ (or equivalently $\Theta \to -1$ as $z \to +\infty$ and $\Theta \to -1$ as $z \to -\infty$) continuity of the stress induced by director deformations implies that $d\Theta/dz = 0$ at $z = 0$.

The first case ($\Theta = 0$ at $z = 0$) is similar to the model of De Meyere *et al.* [10] where the liquid crystal becomes smectic $A$ at the chevron interface while the second case

($d\Theta/dz = 0$ at $z = 0$) is similar to the model of Clark and Rieker. However, as discussed previously, these two models do not include biaxiality.

Given that in the first of these cases there exist large distortions to the smectic cone angle for which our Landau–de Gennes model may be invalid we will subsequently only consider the second case. We will therefore use the following boundary conditions:

$$\Theta \rightarrow 1 \quad \text{as} \quad Z \rightarrow \pm\infty, \tag{22a}$$

$$\sigma \rightarrow 1 \quad \text{as} \quad Z \rightarrow \pm\infty, \tag{22b}$$

$$d\Theta/dz = 0, \quad \sigma = 0 \quad \text{at} \quad Z = 0. \tag{22c}$$

Then due to the symmetry of the system we need only consider the region $z > 0$.

The chevron interface is therefore described by the two coupled nonlinear equations (19) together with the boundary conditions (22). The full equations will be solved numerically using the continuation package AUTO97 [15,16]. However, it is also possible to solve the governing equations analytically under certain simplifying approximations.

When $\lambda = 0$ Eqs. (19) reduce to

$$0 = \frac{d^2\sigma}{dZ^2} - \sigma + \Theta^2, \tag{23a}$$

$$0 = \alpha \frac{d^2\Theta}{dZ^2} + \Theta(1 - \Theta^2). \tag{23b}$$

For the above boundary conditions this has the trivial solution $\Theta = 1$ and $\sigma = 1 - e^{-Z}$ or in dimensional variables,

$$\theta = \theta_e, \tag{24a}$$

$$S = S_e(1 - e^{-z\sqrt{3A/2\kappa}}). \tag{24b}$$

This solution corresponds to the classical analysis of the chevron put forward by Clark and Rieker [7]. In common with their solution, this solution also has the cone angle $\theta_e$ constant throughout the cell, and the director **n** at the chevron interface is positioned at the intersection of the smectic cones from the two halves of the chevron structure. However, as we also introduced the need for continuity of the biaxial order across the chevron interface, this solution to our model additionally has the biaxial ordering *melting* at this internal surface. This is illustrated in Fig. 4.

An interesting feature of our solution is that Eq. (24b) allows us to estimate the width of this melt region. This corresponds to an internal boundary layer thickness or correlation length $z_{\text{BL}}$ given by

$$z_{\text{BL}}^{S} = \left(\frac{2\kappa}{3A}\right)^{1/2}. \tag{25}$$

Provided that the biaxial ordering is indeed driven by the molecular tilt (or cone angle), as we have assumed in deriving the above solutions, and we are well away from any naturally occurring biaxial phase transition (largely a material dependent property), and from the cell surfaces, then this correlation length is largely independent of temperature.

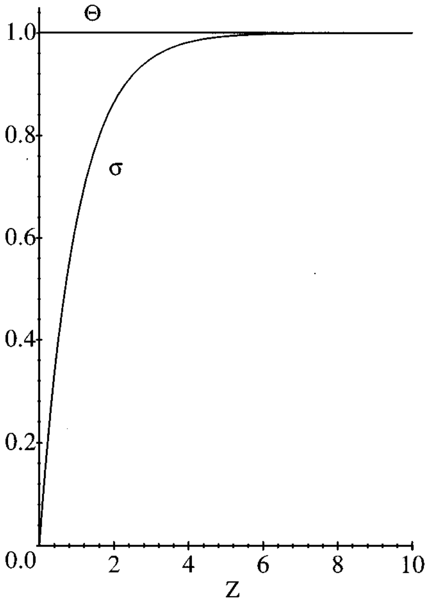

FIG. 4. Analytic solutions for the normalized cone angle $\Theta$ and biaxial order parameter $\sigma$ when $\lambda = 0$.

It should be noted that in practice the condition $\lambda = 0$ implies $A = 0$ or $S_e = 0$, Eq. (17d), and if we assume $A > 0$, the above solution (24b) strictly reduces to $S = 0$ and the nondimensional variable $\sigma$ is undefined. However, the form of $\sigma$ found above will be useful in the following section.

When $\lambda \neq 0$ the equations are not very tractable to an analytic approach. For part of this regime we can make some analytic progress using a perturbative approach when $\lambda \ll 1$. This condition is equivalent to $S_e \ll 1$, i.e., the smectic $C$ phase is weakly biaxial.

Thus using $\lambda$ as a perturbation parameter we assume that

$$\Theta = 1 + \lambda\Theta_1 + O(\lambda^2), \tag{26a}$$

$$\sigma = 1 - e^{-Z} + \lambda\sigma_1 + O(\lambda^2). \tag{26b}$$

Then to first order Eqs. (19) become

$$0 = \frac{d^2\sigma_1}{dZ^2} - \sigma_1 - 2\Theta_1, \tag{27a}$$

$$0 = \alpha \frac{d^2\Theta_1}{dZ^2} - 2\Theta_1 = e^{-Z}, \tag{27b}$$

which must be solved with the boundary conditions

$$\Theta_1^2 = 0, \quad \sigma_1 = 0 \quad \text{as} \quad Z \rightarrow \infty, \tag{28a}$$

$$\frac{d\Theta_1}{dZ} = 0, \quad \sigma_1 = 0 \quad \text{at} \quad Z = 0. \tag{28b}$$

The solutions are

$$\Theta_1 = \frac{1}{\alpha - 2}\left[\left(\frac{\alpha}{2}\right)^{1/2} e^{-Z\sqrt{2/\alpha}} - e^{-Z}\right], \tag{29a}$$

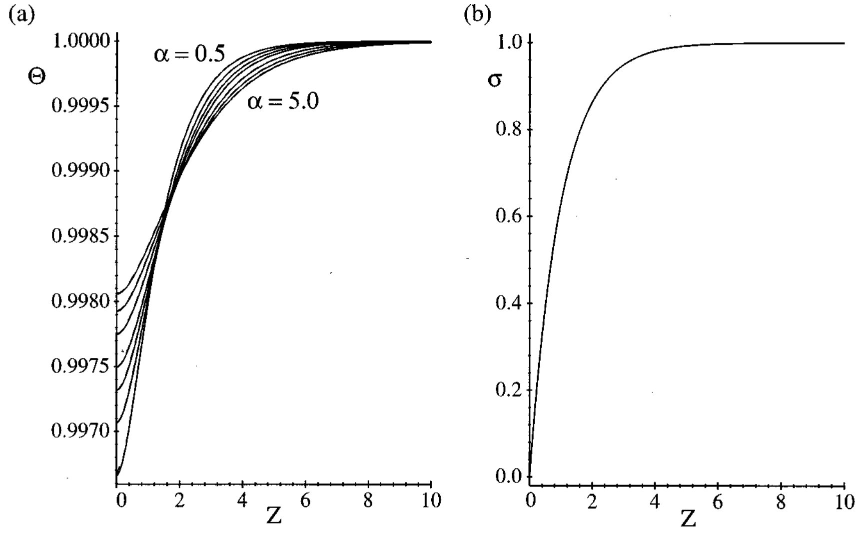

FIG. 5. Comparison between analytical (dashed lines) and numerical (solid line) solutions for (a) Θ and (b) $\sigma$, when $\lambda = 0.01$ and $\alpha = 0.5,1.0,1.5,2.0,3.0,4.0,5.0$.

$$\sigma_1 = \frac{\sqrt{2\alpha^3}}{(\alpha-2)^2}\left(e^{-Z} - e^{-Z\sqrt{2/\alpha}}\right) + \frac{Z}{(\alpha-2)} e^{-Z}, \quad (29b)$$

when $\alpha \neq 2$ and

$$\Theta_1 = \tfrac{1}{4}(1+Z)e^{-Z}, \quad (30a)$$

$$\sigma_1 = -\frac{(3Z+Z^2)}{8} e^{-Z}, \quad (30b)$$

when $\alpha = 2$. These solutions are illustrated in Figs. 5–7. For both $\lambda = 0.01$ and $\lambda = 0.1$ (Figs. 5 and 6) large values of $\alpha$ give larger regions of Θ variation, whereas variations of $\sigma$ are governed by the first order term of Eq. (26b) which, in the nondimensionalized coordinate $Z$, does not vary as $\alpha$ varies. We have therefore found two distinct correlation lengths. In terms of dimensional variables, variations in $S$ are governed by the length scale given by Eq. (25) and variations in $\theta$ are governed by two length scales, $z_{\mathrm{BL}}^{S}$ and

$$z_{\mathrm{BL}}^{\theta} = \frac{1}{\theta_e}\left(\frac{K'}{2b}\right)^{1/2}. \quad (31)$$

For $\alpha > 2$, $z_{\mathrm{BL}}^{\theta} > z_{\mathrm{BL}}^{S}$ while for $\alpha < 2$, $z_{\mathrm{BL}}^{S} > z_{\mathrm{BL}}^{\theta}$.

Figure 7 shows the analytic solutions for larger values of $\lambda$ (when $\alpha = 2$). For large values of $\lambda$, while the region over which Θ varies does not change significantly, there is a much larger reduction in the value of $\Theta(=\theta/\theta_e)$ at the chevron interface. The $\sigma$ profiles in Fig. 7(b) show a slight increase in the chevron interface region for larger values of $\lambda$. At this point it should be stressed that the above analysis is only valid when $\lambda \ll 1$ and consequently as $\lambda$ increases the accuracy of the approximate analytic solutions diminishes.

For the case when $\lambda$ is not small we employed a numerical approach using the continuation package AUTO97 to solve the governing equations (19) with the boundary conditions (22). The solutions are also illustrated in Figs. 5–7. It can clearly be seen from Fig. 5 that the analytic and numerical solutions are very similar for $\lambda = 0.01$. As we would expect, the differences between the two solutions are growing when $\lambda = 0.1$ (Fig. 6). Figure 7 shows that as $\lambda$ increases the difference between the analytic and numerical solutions grows considerably.

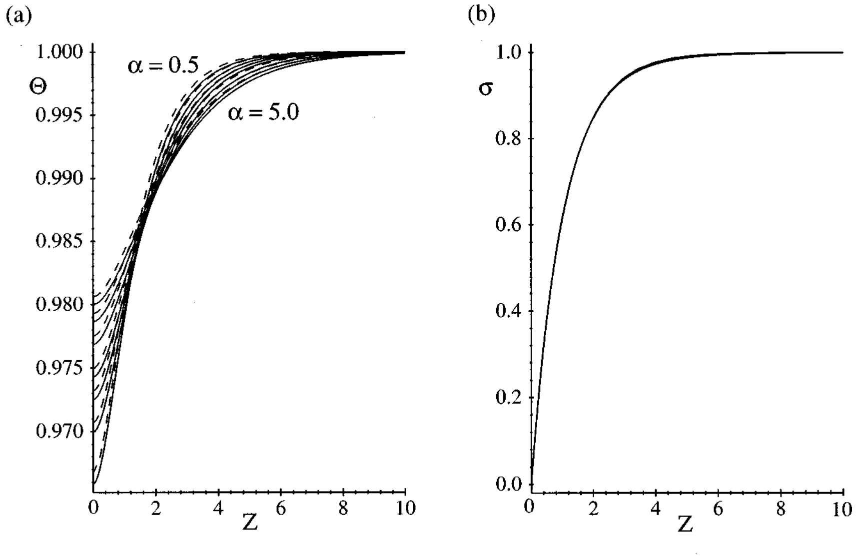

FIG. 6. Comparison between analytical (dashed lines) and numerical (solid line) solutions for (a) Θ and (b) $\sigma$, when $\lambda = 0.1$ and $\alpha = 0.5,1.0,1.5,2.0,3.0,4.0,5.0$.

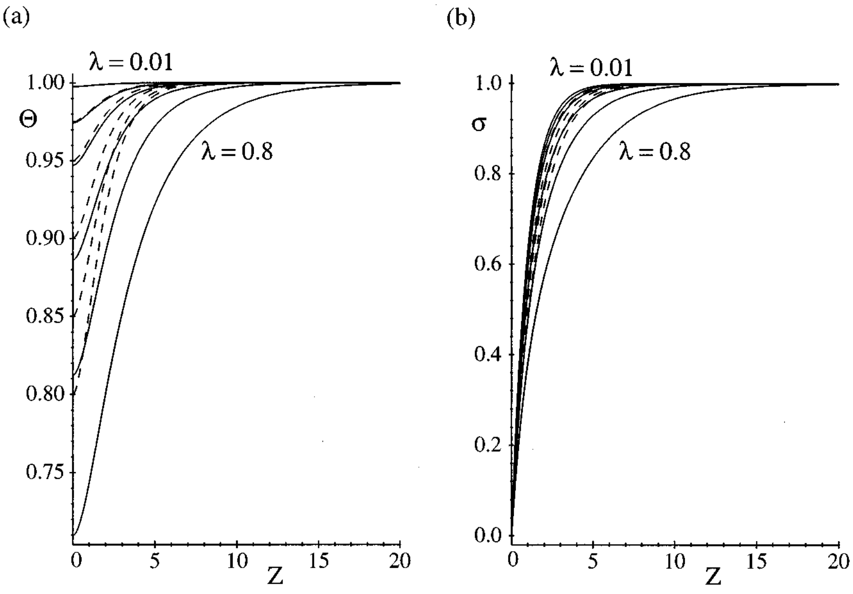

FIG. 7. Comparison between analytical (dashed lines) and numerical (solid line) solutions for (a) $\Theta$ and (b) $\sigma$, when $\alpha = 2.0$ and $\lambda = 0.01, 0.1, 0.2, 0.4, 0.6, 0.8$.

## III. DISCUSSION

We have proposed a model for the chevron interface that is based on the requirement for continuity in the smectic *C* biaxial order parameter *S*, across the chevron tip. In order to make the problem tractable we assume a simple twist deformation in the director **n**. We balance this against the energetic cost of changing the cone angle and the biaxial order around the molecular long axis.

For weakly biaxial $S_C$ materials it was possible to find an analytic expression for the chevron structure. From this solution we determined two characteristic length scales, $z^S_{\mathrm{BL}}$ and $z^\theta_{\mathrm{BL}}$, associated with the thickness of the regions of distortions to the order parameter and cone angle, respectively.

It was found that, while changes in the two system parameters, $\alpha$ and $\lambda$, may significantly affect distortions of the cone angle $\theta$ they have little effect on the region of distortion of the order parameter *S*.

The continuity of biaxial ordering at the chevron interface has an important consequence for chiral smectic *C* materials. In the bulk of a $S_C^*$ liquid crystal there exists a spontaneous polarization due to a permanent molecular dipole. However, the rotational symmetry of the state $S = 0$ implies that there is zero polarization at the chevron interface. This result may be extremely important when considering ferroelectric devices, which switch through the coupling between the spontaneous polarization and an applied electric field.

In the future we hope to include biaxial ordering in a more complete model of the chevron interface.

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