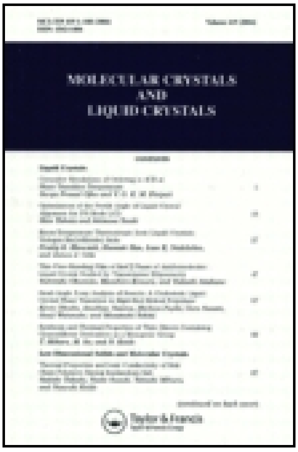

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A Soliton Model for the Chevron Layer Structure in SmC* Liquid Crystals†

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In this work, a simple explanation is given for the chevron layer structure which has been observed in SmC* phase. A phenomenological elastic free energy concerned with layer distortion, *c*-director deformation, and their coupling is proposed to discuss the layer structure of them. It will be shown that there exists a soliton solution corresponding to the chevron structure. The transition layer thickness of the chevron is theoretically estimated as the penetration length (~molecular length)/molecular tilt angle. In similar to the kinked layer structure, the *c*-director rotation angle is also found to show a soliton-like behaviour within the transition region. In addition, the existence of the selective pre-tilt at the bounding surface is explained in the relation with the chevron structure.

Keywords: soliton model, chevron layer structure, SmC liquid crystals*

1. INTRODUCTION

Several material properties of ferroelectric SmC* liquid crystals have been extensively and energetically investigated by many workers in the past decade.[1] Their elastic properties have been also partly clarified on the basis of several different kinds of the elastic free energies.[2–7] In most cases, however, only the director orientation field has been mainly analysed assuming the existence of a flat layer structure. Based on those simplified models, it was found that four kinds of twist states could be stabilised in the surface-stabilised geometry from experimental[8,9] and also theoretical[10] point of views. Moreover, based on the optical observations of the colour difference between the twist states, Shingu et al. explored the existence of the selective pre-tilt of the *c*-director at the surface boundary.[9] However, as far as one supposes the flat layer structure normal to the bounding plates, the origin of the selective pre-tilt could not be understood. Later Ouchi et al. proposed a few models with some kinds of layer structures in order to explain the existence of the pre-tilt and the experimentally observed switching processes in the surface-

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stabilised geometry.[11] Nevertheless, no physical origin of the layer distortion or the inclination with respect to the bounding plates has been clarified yet.

On the other hand, by means of a high resolution X-ray measurement, Clark and Lagerwall first reported an experimental evidence for the existence of several types of distorted local layer structures in the surface-stabilised ferroelectric liquid crystal (SSFLC).[12] Recently, Rieker *et al.* also reported the detailed measurements for a commercial mixture and DOBAMBC (*p*-decyloxybenzylidene-*p'* -amino-2-methylbutyl-cinnamate).[13] They found the chevron layer structure as shown in Figure 1 and an inclined layer structures in SSFLC in consistence with the proposal by Ouchi *et al.*[11] In addition, Ouchi *et al.* confirmed the existence of the selective pre-tilt in the racemate of DOBAMBC.[11] Therefore such layer distortion could be observed not only in SmC* but also in SmC phase. In fact, such a chevron layer structure had been also suggested by Pelzl *et al.* for some SmC liquid crystals.[14] More recently, Ouchi *et al.* clarified the existence of the chevron structure not only in SSFLC states but also in relatively thick samples with a helicoidal structure.[15] This experimental fact suggests that the origin of the chevron must be closely related to the layer distortion energy rather than the *c*-director deformation energy. In addition, from the fact that the layer tilt angle is not critically affected by the sample thickness and the surface treatment of the substrates,[13] such chevron structures are considered to be caused by the bulk properties rather than the anchoring effect. For this kind of chevron structure in SSFLC, Clark and Rieker provided a simple explanation assuming discontinuities of the *c*-director orientation as well as the layer structure at the middle of the sample based on their experimental observations.[16] From a theoretical view-point, however, the origin of such discontinuities has not been clarified yet. From their experimental fact that the profile of the scattered intensity tends to be broadened as the layer tilt decreases with the increasing temperature,[13] we may infer that the chevron structure has a tendency to change in the manner as shown in Figure 2(a) rather than Figure 2(b) with a steeply kinked layer structure.

In this work, we shall explain the above-mentioned chevron structure as a soliton based on a simple elastic theory concerned with the layer distortion as well as the

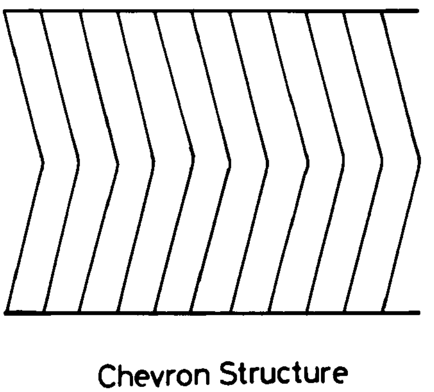

FIGURE 1 Schematic drawing of typical chevron layer structure observed in SmC* phases.[12,13,15,16].

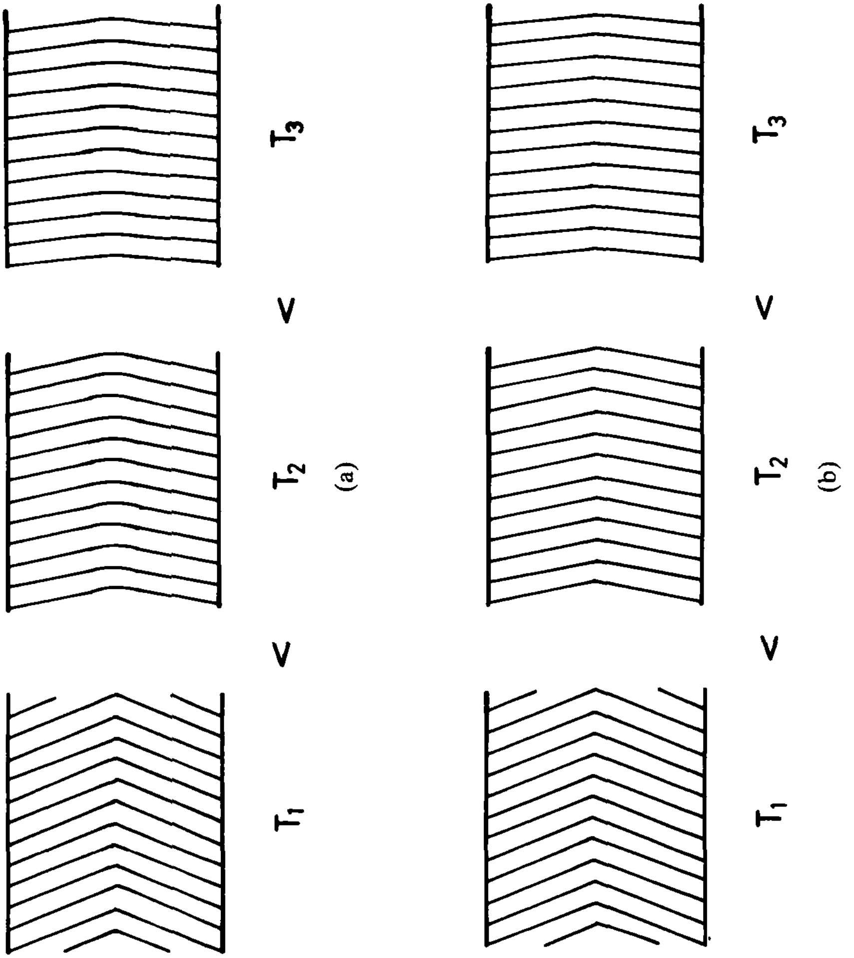

FIGURE 2 (a) Temperature dependence of the chevron layer structures expected by the temperature dependence of the scattered X-ray intensity.[13] (b) Temperature dependence of the chevron layer structure with a steep kink assumed to be independent of temperature change. In this case the width of the scattered X-ray intensity has to be also constant independent of temperature change.

c-director deformation. After solving a coupled differential equation, we shall find a soliton solution corresponding to the chevron structure. Simultaneously the pretilt will be theoretically estimated based on the present soliton model. In Section 2 a simple analysis will be given to explain the chevron structure. Finally Section 3 is devoted to giving a few concluding remarks.

2. MODEL AND ANALYSIS

First of all, let us begin with writing down a phenomenological elastic free energy of SmC* liquid crystals. Suppose that z axis of the Cartesian coordinates as the undistorted layer normal, and that u and Φ are the displacement of layers parallel to z axis and the c-director angle measured from the bounding surface as shown in Figure 3(a) and (b), respectively. Assuming that u and Φ only depend on x perpendicular to the bounding plates, the bulk free energy F of SmC* may be simply put as follows[17,18]

$$F = F_L + F_d + F_c, \tag{1}$$

where F_L (layer distortion energy),[18] F_d (director deformation energy),[6] and F_c (their coupling energy)[17] are defined by

$$F_L = \frac{A}{2}\left[\frac{d^2u}{dx^2}\right]^2 + \frac{B}{8}\left[\left[\frac{du}{dx}\right]^2 - \Theta^2\right]^2, \tag{2}$$

$$F_d = \frac{K}{2}\left[\frac{d\Phi}{dx}\right]^2 + Kq_B \sin\Phi \frac{d\Phi}{dx}, \tag{3}$$

$$F_c = C\frac{d^2u}{dx^2}\frac{d\Phi}{dx}; \tag{4}$$

here A and B are the splay elastic constant and the compression modulus of the smectic layers, respectively, Θ is the molecular tilt angle with respect to the local layer normal, K is an elastic constant for c-director deformation, q_B is the inherent bend wave number, and C is a coupling constant between the layer distortion and the c-director deformation. In addition, Θ is assumed to be constant over the SmC* sample. To simplify the present approach, we restrict ourselves to one-dimensional

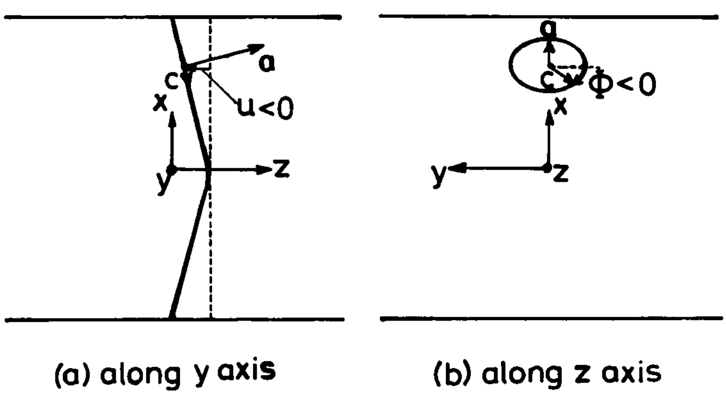

FIGURE 3 Coordinate system and geometry under consideration. Here **a** and **c** are the layer normal unit vector and the c-director, respectively. Φ is the azimuthal angle of the c-director about **a** and measured from $-y$ axis. It is assumed that z axis is coincident with the layer normal in the undistorted state. The relative layer displacement is denoted by u and assumed to be 0 at $x = 0$ or the middle plane parallel to the substrates. In this case, $u < 0$, $du/dx < 0$, $\Phi < 0$ for $x > 0$ and $u < 0$, $du/dx > 0$, $\Phi > 0$ for $x < 0$. (a) The view along y axis. (b) The view along z axis.

problem along x axis as shown in Figure 3(a) and (b). Therein z axis is assumed to be coincident with the layer normal in the undistorted state. This simplification seems to be supported by the experimental observation by Ouchi et al.[15] In fact they observed the chevron structures even in thick (50–350 μm) samples as well as thin (4 μm) samples. This experimental evidence suggests that the origin of the chevron structure is almost independent of the helical structure or the variation of Φ along helical axis. Therefore, as a first approximation, the present one-dimensional model may be accepted to study the origins of the chevron structure and the pre-tilt. Here it may be worthwhile to mention the physical meaning of B term in F_L, which represents a coupling between the molecular tilt and the layer distortion. This term has two minima at $du/dx = \pm\Theta$. That is, this energy shows that when a system goes from SmA to SmC* (or SmC) molecules have a tendency to slide each other rather than rotating to keep their intermolecular distance constant. This type of effect was first pointed out by Ribotta and Durand in a discussion of mechanical instabilities of SmA liquid crystals under an external stress.[18] The physical meaning of B term can be given as follows according to Ribotta and Durand.[18] Suppose that the initial layer thickness d_0 (~molecular length) in SmA phase. Then in SmC phase molecules prefer tilt alignment accompanied by a reduction of the layer thickness from d_0 to $d_0\cos\Theta \simeq d_0\,(1 - \Theta^2/2)$. At the same time, the layer thickness in SmC phase has to be given by $d\cos(\partial u/\partial x) \simeq d\{1 - (\partial u/\partial x)^2/2\}$ when there exists the layer displacement $u(x)$ from the ground state. Therefore, noting that $d\cos(\partial u/\partial x) \equiv d_0\cos\Theta$, the excess free energy accompanied by the above two mechanisms can be given by $(1 - d/d_0)^2 \simeq \{(\partial u/\partial x)^2 - \Theta^2\}^2/4$ which just corresponds to B term in (2).[18] Later, this coupling effect will be found to play an important role to explain the chevron structure.

Integrating F over the sample thickness d along x, the total energy $\langle F\rangle$ per unit area is given by,

$$
\begin{aligned}
\langle F\rangle &= \int_{-d/2}^{+d/2} dx\, F \\
&= A\int_{-d/2}^{+d/2} dx \left[\frac{1}{2}\left[\frac{dv}{dx}\right]^2 + \frac{1}{8\lambda^2}[v^2 - \Theta^2]^2 \right. \\
&\quad \left. + \frac{\kappa}{2}\left[\frac{d\Phi}{dx}\right]^2 + \gamma\frac{dv}{dx}\frac{d\Phi}{dx}\right] \\
&\quad + Kq_B\{\cos\Phi\,(-d/2) - \cos\Phi\,(+d/2)\},
\end{aligned} \tag{5}
$$

where $v(x)$, λ, κ, and γ are defined by

$$v(x) = \frac{du(x)}{dx}, \tag{6}$$

$$\lambda = [A/B]^{1/2}, \tag{7}$$

$$\kappa = K/A, \tag{8}$$

$$\gamma = C/A, \tag{9}$$

respectively; here λ is referred as a penetration length of smectics and of the order of molecular length.[17,18] Minimizing $\langle F\rangle$ with respect to $v(x)$ and $\Phi(x)$, we can derive the following coupled ordinary differential equations,

$$\frac{d^2v}{dx^2} + \gamma\frac{d^2\Phi}{dx^2} + \frac{1}{2\lambda^2}(\Theta^2 - v^2)v = 0, \tag{10}$$

and

$$\kappa\frac{d^2\Phi}{dx^2} + \gamma\frac{d^2v}{dx^2} = 0. \tag{11}$$

Eliminating Φ from Equations (10) and (11), we have

$$\frac{d^2v}{dx^2} + \frac{1}{2\delta\lambda^2}(\Theta^2 - v^2)v = 0, \tag{12}$$

where δ is defined by

$$\delta = 1 - \gamma^2/\kappa = 1 - C^2/(AK) < 1. \tag{13}$$

Integrating (12), one finds

$$\left[\frac{dv}{dx}\right]^2 + \frac{1}{4\delta\lambda^2}\{2v^2\Theta^2 - v^4\} = C_0. \tag{14}$$

According to the experimental observation by Clark and Rieker,[16] we shall assume that $dv/dx = 0$ and $|v| = \Theta$ far from the middle point or $x = 0$. Therefore C_0 results in $\Theta^4/4\delta\lambda^2$). Then assuming $\delta > 0$ to assure the minimization of energy, we have

$$\frac{dv}{dx} = +/- \frac{1}{2\delta^{1/2}\lambda}(\Theta^2 - v^2), \tag{15}$$

and further assuming a solution such that $v(-x) = -v(x)$

$$v(x) = +/- \Theta\tanh\left[\frac{\Theta x}{2\delta^{1/2}\lambda}\right]. \tag{16}$$

This solution corresponds to a single soliton which exists as far as $\delta > 0$. Then integrating Equation (16), we have

$$u = +/- 2\delta^{1/2}\lambda\log\left[\cosh\left[\frac{\Theta x}{2\delta^{1/2}\lambda}\right]\right], \tag{17}$$

where we put $u(0) = 0$. Next, assuming that $\Phi(-x) = -\Phi(x)$ and that $d\Phi/dx = 0$ far from the middle of the sample,[16] we have

$$\Phi = -/+ \frac{\gamma}{\kappa}\Theta\tanh\left[\frac{\Theta x}{2\delta^{1/2}\lambda}\right]. \tag{18}$$

From this expression, if the anchoring effect at the bounding plates is relatively weak as will be mentioned in the next section, the selective pre-tilt may be expressed by $(\gamma/\kappa)\Theta = (C/K)\Theta$. On the other hand, from the symmetry consideration, since C and K have to be proprotional to Θ and Θ^2 for a small Θ, the selective pre-tilt angle may not be so sensitive to the temperature of sample. Finally we shall evaluate $\langle F\rangle$ as follows

$$\langle F\rangle = A\delta\int_{-d/2}^{+d/2} dx\left[\frac{\Theta^4}{4\delta\lambda^2}\right]\operatorname{sech}^4\left[\frac{\Theta x}{2\delta^{1/2}\lambda}\right]$$

$$\simeq \frac{4}{3}A\delta^{1/2}\frac{\Theta^3}{2\lambda}, \tag{19}$$

where we assumed $d >> \delta^{1/2}\lambda/\Theta$. This energy is considered to be the excitation energy of a single soliton corresponding to the chevron. As can be seen from (19), the excitation energy does not include the chiral contribution or q_B. Therefore we may conclude that the present results are not altered even for SmC.[14]

3. CONCLUDING REMARKS

In this paper, we have proposed a soliton model to explain the origin of the chevron structure recently observed by means of the high resolution X-ray measurement.[12,13,15,16] Taking account of the compression and the distortion energies of layers as well as the c-director deformation energy, we found a soliton solution for the layer orientation and the c-director rotation. Based on the present simple model, we may conclude that the chevron layer structure results from the sliding of molecules rather than rotating when the sample is cooled down from SmA to SmC* (or SmC). The thickness of the transition region may be estimated as $\delta^{1/2}\lambda/\Theta \sim 10^{-8}$ m with $\delta \sim 1$, $\lambda \sim 10^{-9}$ m, and $\Theta \sim 0.1$. In addition we may conclude that the transition layer thickness $\delta^{1/2}\lambda/\Theta$ increases with the increasing temperature as shown in Figure 2(a) consistent with the expectation from the experimental observation of the intensity profile of the X-ray analysis.[13] For relatively weak anchoring for the c-director at the boundaries, the selective pre-tilt angle may be estimated by $(\gamma/\kappa)\Theta = (C/K)\Theta$. Finally the excitation energy of the soliton may be estimated as $(2/3)A\delta^{1/2}\,\Theta^3/\lambda \sim 10^{-5}\ J/m^2$ (10^{-2} erg/cm^2) with $A = 10^{-11}\ N$, $\delta \sim 1$, and $\lambda \sim 10^{-9}$ m. Remarkably this excitation energy is comparable with the orientational energy barrier estimated by Clark and Rieker based on their model.[16] Furthermore this excitation energy is also comparable with the typical anchoring energy Γ for n-director between nematics and solids.[19] Since the anchoring energy for the c-director orientation in SmC* (or SmC) phase may be estimated as $\Theta^2\Gamma \sim 0.01\Gamma$, the excitation energy is considered to be much larger than the anchoring energy for the c-director. Therefore, as was previously assumed, the anchoring energy of the c-director can be neglected relative to the bulk energy presently considered. In fact Rieker *et al.* have found that the layer tilt angle is almost independent of the surface treatment and closely related to the molecular tilt angle Θ.[13] Consequently, on the basis of the present soliton model, the selective pre-tilt angle in the chevron structure may be reasonably estimated by $(C/K)\Theta$. In this study, we assumed that the layer tilt angle at the boundaries equals to the molecular tilt angle. While this assumption seems to be plausible from the experimental results for SmC* materials which show SmA-SmC* phase transition.[13] However, it has to be reconsidered for materials which has relatively large molecular tilt angles since Ouchi *et al.* have found that the layer tilt angle is much smaller than the molecular tilt angle for a material, which shows N*-SmC* transition, with a relatively large molecular tilt angle (42 deg: $T - T_c = -10$ K).[15] This point remains to be examined in the future. Moreover, as a further extension of the present approach, it seems to be interesting to generalise the present single soliton model to a multi-soliton one so as to explain two-dimensional walls between two anti-kinked chevrons. Finally it may be worthwhile to note that the present model may predict the chevron structure even in SmA phase if the sample is subjected to an external stress along z axis as has been investigated by Ribotta and Durand for SmA liquid crystals.[18] In such a case, while the term $\Theta^2/2$ in Equation (1) should be replaced by an external stress X along the undistorted layer normal,[18] the approach is formally the same as the present case.

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