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Transitions of Smectic A to Tilted Phases in Thin Free Standing Films of Liquid Crystal

(Peralihan Fasa Smektik A ke Fasa Condong dalam Filem Nipis Hablur Cecair Berdiri Bebas)

CHIA-YUEE LUM, LYE-HOCK ONG* & MOJCA ČEPIC

ABSTRACT

The transition of orthogonal smectic A (SmA) phase to the tilted phases, upon lowering the temperature, is explored with a discrete phenomenological model and the phase diagrams are presented. The results show that the transition of SmA to uniplanar structures can be affected by the effect of chirality. The areas showing the uniplanar phase in the phase diagrams diminish with the increase in effect of chirality.

Keywords: Liquid crystal phase transition; model and theory; thin films

ABSTRAK

Peralihan fasa smektik A (SmA) ke fasa condong hablur cecair, dengan menurunkan suhu, telah dikaji dengan menggunakan model fenomenologi berbentuk diskrit dan gambarajah fasa peralihan ini dipaparkan. Keputusan menunjukkan peralihan fasa SmA ke fasa uniplanar dipengaruhi oleh kesan kekiralan. Luas kawasan untuk fasa uniplanar dalam gambarajah fasa semakin menyusut dengan penambahan kesan kekiralan.

Kata kunci: Filem nipis; model dan teori; peralihan fasa hablur cecair

INTRODUCTION

Thin film smectic liquid crystals offer many fascinating research potentials as the characteristics of thin films vary a lot from the bulk system. Experimental work on freely suspended thin film liquid crystals has been reported earlier (Young et al. 1978) and the work concerns the optical response in thin film smectic C (SmC) liquid crystals. In another experimental study, Rosenblatt et al. (1979) measured the polarization, elastic constant and viscosities of thin film SmC liquid crystals. A few years later, Rosenblatt and Ronis (1981) presented a lattice model to elucidate phase transition properties of thin film liquid crystals.

On the other hand, Landau phenomenological model was used about a decade ago in the studies of uniplanar smectic phases in free-standing films by Rovšek et al. (2000) without the consideration of chirality interaction. This study, include the term due to the effect of chirality in the free energy expression given in (Cepic & Zeks 1995) to investigate the phase transition of thin films from the non-tilted phase to the tilted phase and the phase diagrams are presented in the results.

THE MODEL

The simple phenomenological model presented in Rosenblatt et al. (1981) is modified by including the term due to the chiral interaction of nearest neighbour f, and the free energy density can be shown as:

$$G = \sum_{i=1}^{N} \frac{1}{2}a_0\xi_i^2 + \frac{1}{4}b_0\xi_i^4 + \frac{1}{2}a_1\left(\vec{\xi}_i \cdot \vec{\xi}_{i+1}\right) + \frac{1}{8}a_2\left(\vec{\xi}_i \cdot \vec{\xi}_{i+2}\right) + \frac{1}{2}f\left(\vec{\xi}_i \times \vec{\xi}_{i+1}\right)_z, \quad (1)$$

a_0 and b_0 are the Van der Waals interaction terms. a_0 = $(T - T_0)$ is temperature dependent, where a>0 and is the transition temperature from SmA (orthogonal layered structure) to SmC if only the Van der Waals interaction is considered. a_1 and a_2 are the nearest neighbour (NN) and next nearest neighbour (NNN) interaction terms, respectively. a_1 represents the strength of interaction between $\vec{\xi}_i$ and $\vec{\xi}_{i+1}$ while a_2 gives the strength of interaction between $\vec{\xi}_i$ and $\vec{\xi}_{i+2}$. Positive values of these two terms favour the anticlinic orientations of the molecules while the negative values favour synclinic structures. The chiral term f on the other hand measures the energy related to the molecular chirality which is usually small (Takezoe et al. 2010).

The orthogonal SmA structure is stable when temperature T is higher than T_0. Upon lowering the temperature, SmA structure is energetically less stable. A stable structure at any temperature must fulfill the two conditions that the first derivatives of the free energy in equation (1) with respect to the order parameter must be zero and the second derivatives of the free energy in equation (1) must be positive. The second condition is fulfilled by solving for the positive eigenvalue solutions from the Hessian matrix formed. In this case, as the projection is on a 2D smectic plane, the order parameter $\vec{\xi}_i$ can thus be further dissolved into $\vec{\xi}_{i,x}$ and $\vec{\xi}_{i,y}$ representing the order parameter components into the *x*- and *y*- planes, respectively. The stability limit of the SmA structure is reached when the one of the all positive eigenvalues reaches zero, indicating a phase transition. If there are no other interactions except the Van der Waals interaction, then transition will occur at $T = T_0$, which will give $a_0 = 0$. With the other terms considered, transition temperature of the smectic phase is higher then T_0, giving $a_0 > 0$.

To find structures below the critical SmA-temperature, a numerical procedure as follow is conducted. Initial solutions for the first derivatives of free energy are assumed to be a fraction of the eigenvectors that corresponds to the zero eigenvalue. New solution is assumed to be the initial solution minus a small unknown correction. By linearizing the first derivatives in term of the corrections and equating them to the first derivatives, we solve the 2N linear equations to get the corrections, where N is the layer number and then the approximate solutions can be obtained. Finally, these approximate solutions are substituted as the initial solutions of the system in the second iteration. The iteration proceeds until the approximate solutions have reached the desired precision and these solutions are considered as final solutions.The first derivatives of eq. (1) with respect to $\vec{\xi}_{i,x}$ and $\vec{\xi}_{i,y}$ are, respectively:

$$\frac{\partial G}{\partial \xi_{i,x}} = a_0\xi_{i,x} + b_0\left(\xi_{i,x}^3 + \xi_{i,x}\xi_{i,y}^2\right) + \frac{1}{2}a_1\left(\xi_{i-1x} + \xi_{i+1,x}\right) + \frac{1}{8}a_2\left(\xi_{i-2,x} + \xi_{i+2,x}\right) + \frac{1}{2}f\left(-\xi_{i-1,y} + \xi_{i+1,y}\right), \quad (2)$$

$$\frac{\partial G}{\partial \xi_{i,y}} = a_0\xi_{i,y} + b_0\left(\xi_{i,y}^3 + \xi_{i,y}\xi_{i,x}^2\right) + \frac{1}{2}a_1\left(\xi_{i-1y} + \xi_{i+1,y}\right) + \frac{1}{8}a_2\left(\xi_{i-2,y} + \xi_{i+2,y}\right) + \frac{1}{2}f\left(\xi_{i-1,x} - \xi_{i+1,x}\right). \quad (3)$$

Results and Discussion

From the numerical results obtained, structure after critical SmA is either the synclinic ferroelectric SmC structure, an anticlinic antiferroelectric SmC_A structure or a structure of mixture of synclinic and anticlinic which are simply named the uniplanar structures (Rovsek et al. 2000). With further decrease of temperature, the uniplanar structure slowly destabilizes and eventually evolves into the helical SmCα. Unlike the case where chirality is not considered, there is no second zero eigenvalue observed numerically.

In the case where chirality term is added, the uniplanar regions in the phase diagram (including SmC and SmC_A) shrink as chirality tends to introduce a helical structure. This can be seen by comparing Figure 1(a) with Figure 1(b) for the 3-layered structure and also Figure 2(a) with Figure 2(b) for the 4-layered structure, respectively. In addition, the effect of chirality increases the transition temperature of the uniplanar line. This is most obvious at the value of $a_1/a_2 = 0$. The phase diagrams for the 3-layered structure and the 4-layered structure are significantly different for the same value of *f*. For small values of a_1/a_2, the uniplanar phase evolves into the Sm C_a phase when the temperature $T \rightarrow T_0$. Though the contribution of the chiral term to the free energy can be small, but it has shown that the effect of chirality has significant effect on the phase stability of the 3-layered and 4-layered structures. In general, chirality is an effect which exists in tilted layered structure liquid crystals; and hence this study is an improvement on the understanding of the phase variations with respective to temperature and layer interactions.

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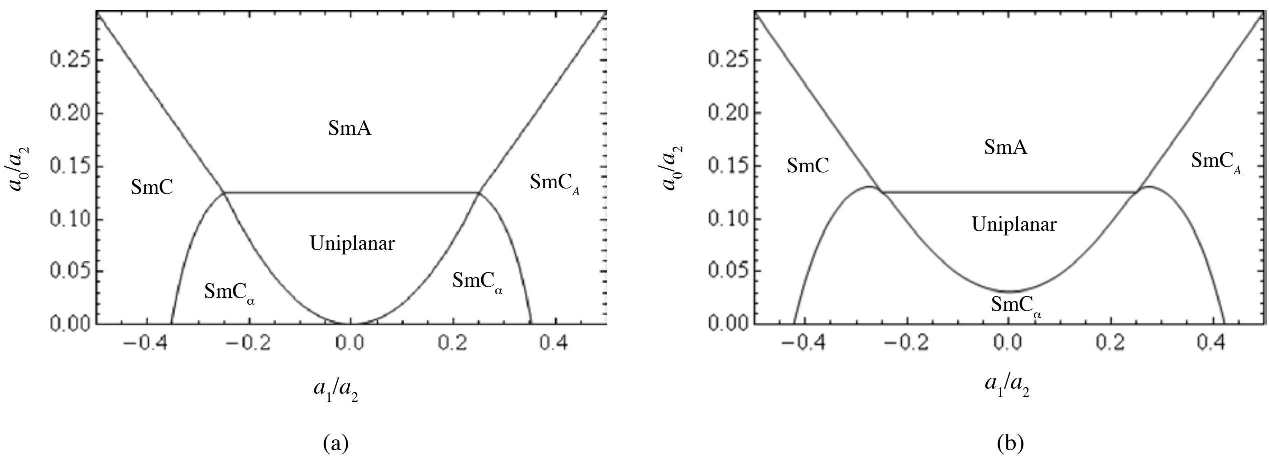

FIGURE 1. (a) Phase diagram of $N = 3, f = 0$ and (b) phase diagram of $N = 3, f = 0.00001$

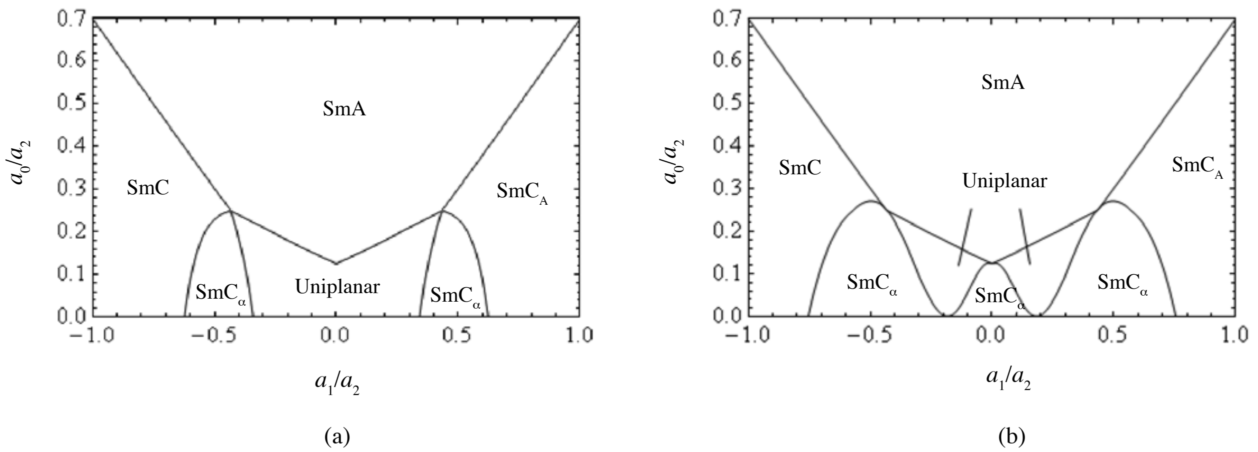

FIGURE 2. (a) Phase diagram of $N = 4, f = 0$ and (b) phase diagram of $N = 4, f = 0.00001$

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Chia-Yuee Lum & Lye-Hock Ong*
School of Physics
Universiti Sains Malaysia
11800 USM, Penang, Malaysia

Mojca Čepic
Faculty of Education
University of Ljubljana
Kardeljeva pl. 16, 1000 Ljubljana, Slovenia

*Corresponding author; email: onglh@usm.my

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