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Formation of Edge Dislocations in the Surface Constrained Smectic a Film

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Formation of Edge Dislocations in the Surface Constrained Smectic a Film

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We study surface driven formation of a lattice of edge dislocations in the SmA phase in the semiinfinite geometry using Landau-Ginsburg phenomenological approach and estimate the conditions where the dislocation structure is stable over the tilted structure and the threshold for the formation of an edge dislocation on increasing the surface positional anchoring strength W_p. The detail structure of an edge dislocation is numerically studied as a function of W_p.

Keywords: SmA liquid crystals; edge dislocations; defects

1 Introduction

We study the structure and surface driven formation of edge dislocation[1] in the SmA liquid crystal (LC) phase in the semiinfinite planar geometry. The geometry of the problem is depicted in Fig.1a. Smectic layers are running along the z-direction and are set perpendicular to the limiting substrate positioned at x=0. We consider the case where L_x, L_y and $L_z \to \infty$, where L_i is the linear size of the sample along

the i-th cartesian coordinate. The substrate enforces the tangential orientational ordering and periodicity $q_s = 2\pi/d_s$ which differs from the thermodinamically stable bulk SmA periodicity $q_o = 2\pi/d_o$ realised at the temperature T. The surface periodicity is due to the memory effect.[2] It was established and memorized at the first contact between the periodic LC phase and the substrate on cooling from the nematic phase (i.e. $q_s \approx q_o(T = T_{NA})$ where T_{NA} stands for the temperature of the nematic-SmA phase transition).

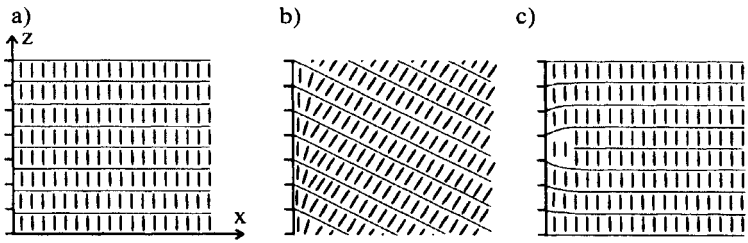

Figure 1: (a) The geometry and coordinate system of the problem. (b) The tilted and (c) the dislocation structure.

The resulting imposed strain on smectic layers can be relieved in different ways. Two possible scenaria considered in this contribution are shown in Figs.1b,c. For $d_s/d_o > 1$ the strain can be relaxed by tilting[3, 4] the layers for $\vartheta = \arccos(d_o/d_s)$. The other option involves the lattice of edge dislocations.[4] In both scenaria far from the limiting surface the equilibrium SmA structure is obtained. Henceforth we name these profiles the TILTED and the DISLOCATION structure. If $d_s/d_o < 1$ only the second scenario is possible.

In this contribution we first estimate the condition for which the dislocation structure is stable. We estimate critical conditions for formation of an edge dislocation increasing the surface positional strength W_p. Then we numerically follow the detail structure of an edge dislocation as a function of W_p.

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2 Theory

We describe the LC ordering in the SmA phase with the nematic director $\vec{n}$ and the smectic complex order parameter $\psi = \eta e^{i\phi}$.[1] The unit vector $\vec{n}$ points along the average orientation of a rodlike LC molecule. The translational order parameter η describes the degree of smectic ordering and ϕ determines the position of smectic layers.

The free energy of the system is given by[1, 4]

$$F = \iiint (f_e^{(n)} + f_h^{(s)} + f_e^{(s)}) d^3r + (f_o^{(n)} + f_p^{(s)}) d^2r. \tag{1}$$

The volume contribution consists of the nematic elastic ($f_e^{(n)}$), smectic homogeneous ($f_h^{(s)}$) and smectic elastic contribution ($f_e^{(s)}$):

$$f_e^{(n)} = \frac{K}{2}\left(\left(\nabla\cdot\vec{n}\right)^2 + \left(\nabla\times\vec{n}\right)^2\right), \tag{1.a}$$

$$f_h^{(s)} = a(T - T_{NA})\,|\psi|^2 + b\,|\psi|^4, \tag{1.b}$$

$$f_e^{(s)} = C\,|\,(\vec{n}\,.\nabla - iq_o)\psi\,|^2 + C\,|\,(\vec{n}\times\nabla)\psi\,|^2. \tag{1.c}$$

The elastic terms are written in the single nematic and smectic elastic approximation in terms of the effective nematic (K) and effective smectic (C) elastic constant. The quantities a, b are LC material constants. Below T_{NA} the bulk smectic ordering is given by $\eta_b = \sqrt{\frac{a(T_{NA}-T)}{2b}}$.

The surface contribution consists of the nematic orientational anchoring ($f_a^{(n)}$) and the smectic positional anchoring term ($f_p^{(s)}$):[1, 5, 6]

$$f_a^{(n)} = -\frac{W_o}{2}\left(\vec{n}\cdot\vec{e_z}\right)^2, \tag{1.d}$$

$$f_p^{(s)} = W_p\left|\psi - \psi_p\right|^2. \tag{1.e}$$

The surface terms included in the model mimic the orientational and positional anchoring weighted by the anchoring constants W_o and W_p, respectively. $\vec{e_z}$ is the unit vector along the z-coordinate and ψ_s is the smectic ordering enforced by the surface. Henceforth the strong orientational anchoring is assumed (i.e. $W_o \to \infty$).

The characteristic lengths[1] relevant for our study are the smectic correlation length $\xi = \sqrt{C/(a \mid T - T_{NA} \mid)}$, the nematic penetration length $\lambda = \sqrt{K/(Cq_o^2\eta_b^2)}$, and the smectic surface extrapolation length $d_s = C/W_p$. It is also convenient to introduce the dimensionless layer stress $\varepsilon = 1 - d_o/d_s$ and the reduced temperature $\tau = (T - T_{NA})/T_{NA}$.

We consider the case where the SmA structure exhibits variations only in the (x,z) plane. The director field is parametrized as $\vec{n} = \vec{e}_x \sin\vartheta + \vec{e}_z \cos\vartheta$ where the unit vector $\vec{e}_i$ points along the i-th cartesian coordinate. The variational parameters ϑ, η and ϕ depend only on x and z.

3 Results

3.1 Analytic estimates

We first consider the case $d_s/d_o > 1$ and estimate the regime where the dislocation structure is stable with respect to the tilted one.

In the tilted structure the LC molecules suffer the nematic splay deformation at the surface extending roughly over the distance λ. We further assume $d_s/d_o \approx 1$ so that $\vartheta << 1$. Taking into account $\mid \nabla.n \mid \approx \vartheta/\lambda \approx \sqrt{2\varepsilon}/\lambda$ and that smectic and nematic elastic penalties are similar (this is evident from the definition of λ) one finds

$$G_t = \frac{F_t}{L_y L_z} \approx 2\varepsilon K/\lambda \tag{2}$$

as an estimate for the free energy F_t of the tilted structure.

To estimate the free energy costs of the dislocation structure we assume that the core of an edge dislocation is essentially nematic and that it extends over the distance given by ξ. The penalty for melting is roughly given by $\mid f_b^{(s)} \mid \pi\xi^2 L_y = \pi C\eta_b^2 L_y/4$. Taking into account $\mid \nabla\eta \mid \approx \eta_b/\xi$ one gets the estimate for the free energy of the dislocation structure in the following way

$$G_d = \frac{F_d}{L_z L_y} \approx \frac{5}{4}\pi C\eta_b^2 n_{edge} \approx \frac{5}{4}\pi C\eta_b^2 \varepsilon/d_o. \tag{3}$$

Here n_{edge} describes number of edge dislocations per distance L_z. Therefore the dislocation structure is thermodynamically stable if

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$G_d < G_t$ yielding the condition

$$\frac{16}{5}\lambda q_o = \frac{16}{5}\sqrt{\frac{K}{C\eta_b^2}} > 1. \tag{4}$$

As expected the dislocation structure is preferred close to the phase transition where smectic melting is relatively chip. At lower temperatures the dislocation structure can be, e.g., stabilized with an external electric field $\vec{E}$ pointing in the z-direction for the positive dielectric anisotropy $\Delta\chi$. The difference between the field free energy contribution of dislocation and the tilted structure is roughly $\Delta G \approx -\frac{KL_x\vartheta^2}{2\xi_E^2}$ where ξ_E is the electric field correlation length. Therefore in the semiinfinite geometry ($L_x \to \infty$) for a finite value of $\vec{E}$ this term always stabilizes the dislocation structure with respect to the tilted one.

In the following we consider the case where the condition for the stability of the dislocation structure is fulfilled. We estimate value of W_p where edge dislocations depin from the surface. In order to do this we compare the free energy cost per unit surface L_yL_z of the edge dislocations formed at the surface ($G_d^{(surf)}$) and in the bulk ($G_d^{(bulk)}$). The latter was already estimated in eq.(3) i.e. $G_d^{(surf)} = G_d$. In estimating $G_d^{(surf)}$ we assume that the surface cuts half of an dislocation yielding the bulk contribution of the order $G_d/2$. The presence of dislocations at the surface introduces also the contribution from the positional anchoring term. Assuming that the surface enforces $\eta_s = \eta_b$ one finds

$$G_d^{(surf)} \approx (\frac{5\pi}{8}C\eta_b^2 + 2\xi W_p)n_{edge}. \tag{5}$$

In order that the edge dislocation depins from the surface the condition $G_d^{(surf)} > G_d^{(bulk)}$ has to be fulfilled yielding

$$\frac{8}{5\pi}\frac{\xi}{d_p} = \frac{8}{5\pi}\frac{W_p\xi}{C} > 1. \tag{6}$$

3.2 Numerical results

In order to get quantitative information about the depinning phenomenon we perform the numerical minimization of Eq.(1). We fo-

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cus to the formation of an edge dislocation and its depinning from the surface while increasing the positional anchoring strength.

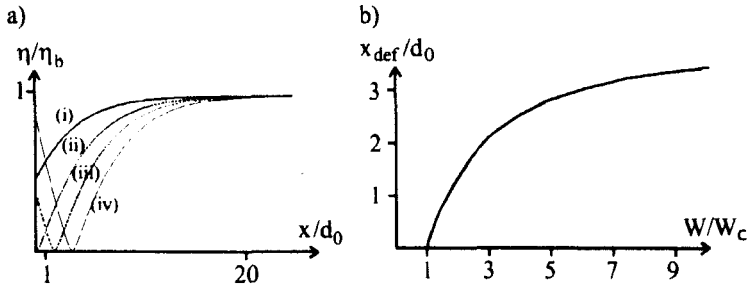

Figure 2: (a) The spatial profile $\eta = \eta(x)$ at the soliton wall. $\varepsilon = 0.05$, $\tau = -0.05$,(i) $W_p/W_c = 0.5$, (ii) $W_p/W_c = 1$, (iii) $W_p/W_c = 3$, (iv) $W_p/W_c = 10$. (b) The position of the edge dislocation as a function of W_p/W_c.

In Fig.2a we plot spatial dependence of the order parameter at the soliton wall (the (x,y) plane through the edge dislocation) for different values of W_p. The edge dislocation is formed when the order parameter drops to zero. The position x_{def} of the dislocation as function of W_p is given in Fig.2b. It is formed at $W_c = W_p$ and it saturates roughly at ξ from the wall for $W_p/W_c > 10$. The structural details of the edge dislocation for various ratios W_p/W_c are shown in Fig.3.

4 Conclusions

We have studied the surface driven formation of edge dislocations in the SmA liquid crystal. The driving mechanism is the mismatch between the periodicities introduced by the smectic elasticity and surface positional anchoring. For $d_o/d_s < 1$ the imposed strain can be relieved also by tilting the layers for $\vartheta = \arccos(d_o/d_s)$. In this regime the dislocation structure is stable with respect to the tiled one provided $3\lambda q_o > 1$. For $d_o/d_s > 1$ the tilted scenario is not possible. In the dislocation structure the edge dislocation depins from the surface if $\xi/(2d_p) > 1$. In order to get quantitative insight into the

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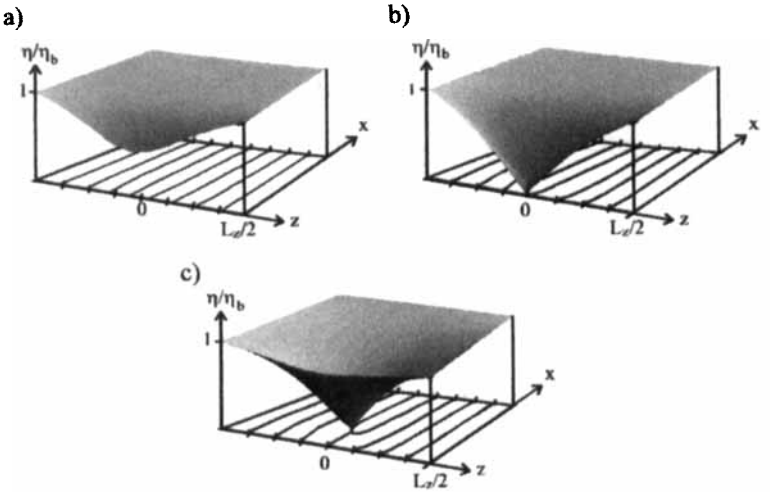

Figure 3: The spatial profile $\eta = \eta(x, z)$ of an edge dislocation for (a) $W_p/W_c = 0.5$,(b) $W_p/W_c = 1$,and (c) $W_p/W_c = 5$. $\varepsilon = 0.05$, $\tau = -0.05$. See Color Plate VIII at the back of this issue.

problem we numerically simulated the formation and depinning of the edge dislocation on increasing the surface positional strength. The dislocations is formed close to the surface at $W_p = W_c$ and it saturates at the distance given by ξ from the wall. We find that the ratio x_{def}/d_o scales with W_p/W_c.

4.0.1 Acknowledgement

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