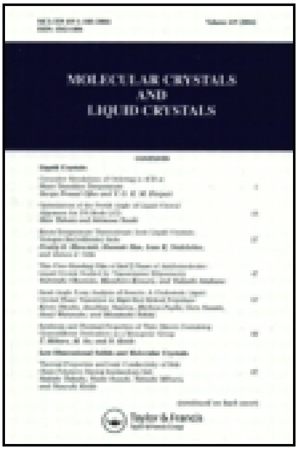

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Short Pitch Smectic Structures in Electric Field

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When an external electric field is applied to short pitch polar smectics, their helical structures distort and unwind. The final transition to completely unwound structure can be continuous or discontinuous. Within the discrete phenomenological model the nature of the transition depends on the existence of the next-nearest neighboring layers interactions. If they are present, the transition is discontinuous. We try to elucidate this phenomenon.

Keywords: antiferroelectric liquid crystals; discrete model; electric field

INTRODUCTION

We consider the influence of the external electric field E on the helical structure of the polar short pitch smectic C_α^* phase within the discrete phenomenological model [1]. Order parameter is a set of tilt vectors ξ_i, where ξ_i is a projection of the nematic director n_i in i-th layer onto the smectic plane. The part of the free energy which accounts for inter-layer interactions up to the next-nearest neighbors and interactions with external field is written in a

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simple form:

$$G_{il} = \sum_i \left[\frac{1}{4}a_1(\xi_{i-1}\cdot\xi_i + \xi_i\cdot\xi_{i+1}) + \frac{1}{4}f(\xi_{i-1}\times\xi_i + \xi_i\times\xi_{i+1}) + \frac{1}{16}a_2(\xi_{i-2}\cdot\xi_i + \xi_i\cdot\xi_{i+2}) - \boldsymbol{E}\cdot\boldsymbol{P}_i\right]. \tag{1}$$

Indispensable terms in free energy take into account achiral (a_1) and chiral (f) nearest neighboring layers interactions and achiral next-nearest layers interactions (a_2). External electric field E is parallel to the smectic layers and couples to a ferroelectric polarization of each smectic layer $P_i = (\xi_i \times n_0)P_0 D$, where n_0 is the smectic layer normal and D is the smectic layer thickness. Polarization P_i is parallel to the smectic layer and perpendicular to the tilt. Tilt vector can be described by the magnitude θ_i and the phase angle of the tilt ϕ_i. We do not consider variations of the magnitude of the tilt with electric field, θ_i is taken to be the same in all the layers and constant, $\theta_i = \theta_0$. The magnitude of the polarization P_i is therefore also constant.

When the field is zero ($E = 0$), minimization of the free energy (1) gives the zero-field short pitch helical structure of the smectic C_α^* phase, if nearest and next-nearest layers interactions are competing. Reasonable choice for the model parameters is $a_1 > 0$ and $a_2 < 0$ [1]. Chiral interactions suppress degeneracy between two handedness. The pitch p_0 of the helical structure of the smectic C_α^* phase is defined by a relation between the model parameters

$$f = a_1 \tan\alpha_0 + a_2 \sin\alpha_0. \tag{2}$$

The angle α_0 describes the phase angle variations of the tilt from one layer to the next, $\phi_{i+1} = \phi_i + \alpha_0$. The pitch is related to α_0, $p_0 = 2\pi D/\alpha_0$. Since parameters a_1, a_2 and f can have in general any rational values, also the pitch p_0 is in general incommensurate with the smectic layer thickness. It is relevant to say, that the same zero-field pitch can be obtained choosing different combinations of model parameters.

If the field is not zero minimization of the bulk free energy (1) leads to an infinite set of coupled equations

$$\frac{1}{2}a_1[-\sin(\phi_i - \phi_{i-1}) + \sin(\phi_{i+1} - \phi_i)] + \frac{1}{2}f[\cos(\phi_i - \phi_{i-1}) - \cos(\phi_{i+1} - \phi_i)] + \frac{1}{8}a_2[-\sin(\phi_i - \phi_{i-2}) + \sin(\phi_{i+2} - \phi_i)] + \frac{EP_0D}{\theta_0}\sin\phi_i = 0. \tag{3}$$

We solved the system of Eqs. (3) numerically. First, the equations were linearized around the zero-field solution and then solved iteratively for larger and larger fields, the method is described elsewhere [2]. In the presence of electric field the helical structure distorts. The pitch increases with field and within one pitch the tilts reorient, so the average polarization is in direction of the field and also increases with field. In Figure 1 an example of the deformed structure is shown.

Here we concentrate on a particular result: we found, that the nature of the final transition to unwound structure at the critical field E_d depends on the value of parameter a_2, describing the next-nearest layers interactions. When the field is approaching the critical field for the complete unwinding (which is finite in all cases) the pitch extends over an integer number of smectic layers and further increases in steps of one layer [2]. If $a_2 = 0$ the unwinding is found to be continuous, or better said, quasi-continuous: the pitch grows to infinity in steps of one layer. For $a_2 \neq 0$ the final transition is discontinuous – from some finite final pitch of N layers ($p(E_d) = ND$, N is

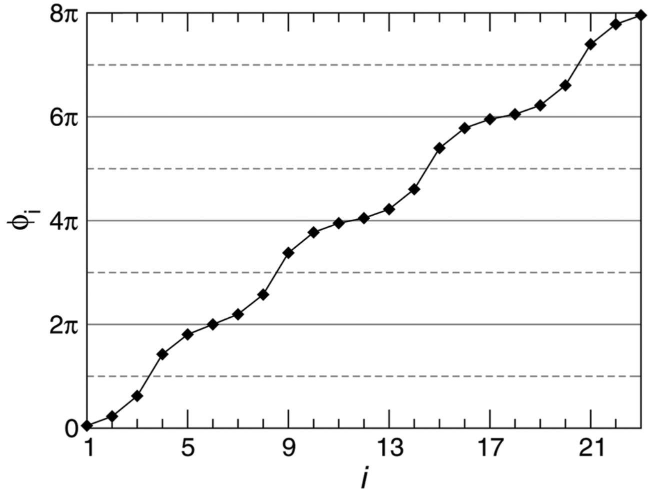

FIGURE 1 Commensurate period of the structure with the pitch $p(E)/p_0 = 1.15 = 23/4$ in electric field, whith $p_0 = 5$ layers. Commensurate period consists of 23 smectic layers and is formed from three subperiods of six layers and one subperiod of five layers. Molecules tend to reorient so the polarization is parallel to the field as much as possible. Phase angle ϕ_i is the angle between external field and polarization in i-th layer. All domain walls (where $\phi_i = \pi, 3\pi, 5\pi, \ldots$) are alike and lengths of all subperiods within commensurate period differ at most for one layer.

integer) to infinity. The larger a_2, the smaller the critical field E_d and shorter the final pitch $p(E_d)$ before unwinding, as can be seen in Figure 2.

To explain the phenomenon, we go back to the bulk free energy describing the zero-field undistorted structure. When we insert the solution for the zero-field helical structure $\theta_i = \theta_0$ and $\phi_i = \phi_0 + i * \alpha$ back into the expression for the free energy, we obtain

$$G(\alpha) = \theta_0^2 \sum_i \left[\frac{1}{2} a_1 \cos\alpha + \frac{1}{2} f \sin\alpha + \frac{1}{8} a_2 \cos 2\alpha\right] \tag{4}$$

when $E = 0$. With only the nearest neighbours interactions (when $a_2 = 0$) the free energy $G(\alpha)$ is symmetric around the minimum as can be seen from a solid curve in Figure 3.

The minimum defines the equilibrium α_0. Due to the symmetry around the minimum the energy costs for additional uniform twisting or unwinding of the helix for the same $\Delta\alpha$, where $\alpha \to \alpha_0 \pm \Delta\alpha$, are the

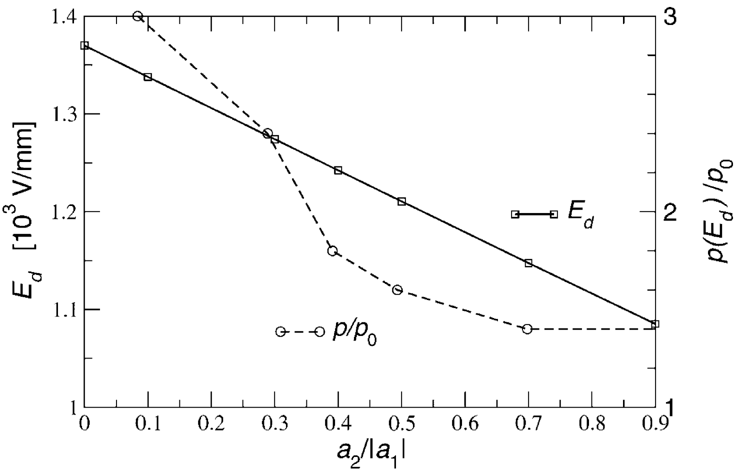

FIGURE 2 Here it is shown, how the critical field E_d and the final pitch $p(E_d)$ depend on the parameter a_2. We take few combinations of parameters $a_2/|a_1|$ and $f/|a_1|$ which all lead to the same zero-field pitch $p_0 = 5$ layers and therefore the same zero-field structure. The structures however unwind differently when electric field is applied. If $a_2 = 0$ (and $f/|a_1| = -3.08$) the structure unwinds quasi-continuously. If $a_2 \neq 0$ (if $a_2/|a_1| = 0.3$, $f/|a_1| = -2.79$ and so on, see Eq. (2)) the complete unwinding occurs at smaller critical field E_d and the pitch jumps from finite $p(E_d)$ to infinity. Material parameters, that led to meaningful values of the critical electric field, were taken from [3]: $P_0 = 100\,\mathrm{nC/cm^2}$, $\theta_0 = \pi/20$ and $a_1/a = -1\,\mathrm{K}$ where $a = 4 \times 10^4\,\mathrm{J/m^3}$.

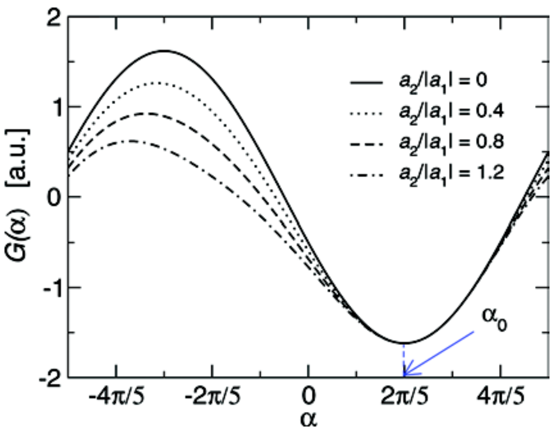

FIGURE 3 Plot of the zero-field bulk free energy $G(\alpha)$, for $p_0 = 5$ layers, which lead to $\alpha_0 = 2\pi/5$. Appropriate value of parameter $f/|a_1|$ can be obtained from Eq. (2).

same. A balance between the elastic forces, stabilizing the helical structure, and electrostatic forces, stabilizing the unwound structure, is in the absence of next-nearest layers interactions obviously achieved in continuous distortion and unwinding of helical structure in electric field until it is unwound completely.

If $a_2 \neq 0$, the symmetry around the minimum is lost. In general, unwinding becomes energetically cheaper. This is apparent from dashed curves $G(\alpha)$ for $a_2 > 0$ in Figure 3, which are less steeper on the side towards $\alpha = 0$. It is more favorable to unwind then to twist, therefore the unwound regions grow faster with field, and the domain walls can also become wider. A consequence is a discontinuous jump to completely unwound planar structure at some critical field E_d. Being given the zero-field structure with certain pitch p_0, the critical field for a discontinuous transition to unwound structure is smaller for larger values of a_2, as can be observed from Figure 2.

To conclude: Whether the ultimate transition to unwound state at E_d occurs at certain finite or diverging pitch, crucially depends on the next-nearest neighbors interactions. If a_2 is zero, the pitch diverges at E_d. If $a_2 > 0$, the pitch of deformed helix is finite at E_d, and a transition to unwound state is discontinuous. If electroclinic effect was not neglected, variations of magnitude of the tilt in electric field could mask the described behavior, which should be checked by more detailed analysis. Nevertheless we believe, that experimental observations of unwinding of the smectic C^*_α short pitch structure in electric field by means of several techniques [4,5] would lead to determination of the ratio f/a_2.

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