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A study of two dimensional smectic layer structure

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In this paper, an analysis of two dimensional smectic layer structure is presented to clarify the layer distortion between two chevrons directed towards opposite directions. From numerical computations, it is found that a parallelogram region appears between two antiparallel chevrons for a sufficiently large molecular tilt and thick sample. The elastic free energy density is found to concentrate near the boundaries of the kinks of the layer structure. In addition the field effect on such a pair of chevrons is presented to show that it is efficient to apply an electric field so as to obtain a quasi-bookshelf structure.

1. Introduction

In recent years, ferroelectric liquid crystals have been extensively studied because of their attractive potential for use in fast electrooptic devices. In spite of much effort by earlier work, there are many unanswered questions. One problem is the difficulty of obtaining a uniform mono-domain sample which is the ideal state of ferroelectric liquid crystals for use in display devices. It is thought the difficulty is related more or less to the chevron layer structure which was first experimentally found by Clark and Lagerwall [1]. It is well appreciated that the existence of chevron layer structures is closely related to the zig-zag defect which can be observed in the surface stabilized sample [2]. Therefore it seems to be worthwhile to analyse the boundary corresponding to the zig-zag defect.

From a theoretical aspect, the elastic free energy of compressible smectics was formulated by Nakagawa [3] recently extending that of incompressible smectics [4]. Based on his theory, the chevron layer structure in the S_C^* phase was analysed within a framework on a one dimensional problem [5–7]. From earlier work, the chevron structure was found to be explained as a kink solution corresponding to a soliton as encountered in non-linear physics [8]. Some extensions of Nakagawa's theory have been reported recently in order to analyse a higher non-linearity of the compression energy and the anchoring force at the bounding plates in a surface stabilized geometry [9, 10]. From previous elastic analysis of chevrons, their one dimensional property has been considerably well understood from a theoretical aspect. Experimentally, however, we encounter often two or three dimensional problems of interest. In fact the previously mentioned zig-zag defect is one of the unsolved fascinating problems based on the elastic theory of compressible smectics.

Here, we analyse two dimensional chevrons and present the effect of the electric field on the domain boundary. In § 2 the theoretical background will be given. Then some numerical results will be shown in § 3. Finally in § 4 we present some concluding remarks.

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2. Theory

In this section we present a set of non-linear equations to analyse the domain boundary between the chevrons.

The elastic free energy density can be phenomenologically expressed by means of a normalized wave vector $\mathbf{a}$, whose modulus $|\mathbf{a}|$ equals 1 in the S_A phase, and a $\mathbf{c}$ director as follows [3]:

$$F=\frac{A}{2}\mathbf{a}_{i,i}\mathbf{a}_{j,j}+\frac{L}{2}(|\mathbf{a}|-\mathbf{a}_0)^2+\frac{B}{2}\mathbf{c}_{i,j}\mathbf{c}_{i,j}-C\cdot\mathbf{a}_{i,i}\mathbf{c}_{j,j}-\mathbf{P}_s\cdot\mathbf{E}, \tag{1}$$

where A, B, C and L are the elastic moduli for the layer distortion energy, for the $\mathbf{c}$ director deformation energy, for splay–splay coupling energy, and for layer compression energy, respectively, $\mathbf{a}_0$ is the equilibrium value of $|\mathbf{a}|$, $\mathbf{P}_s$ is the spontaneous polarization, $\mathbf{E}$ is the electric field and is assumed to be constant in the present framework.

Now, assuming the two dimensional problems in the coordinate system as shown in figure 1 and the electric field along the y axis, we have

$$\begin{aligned}F=&\frac{A}{2}\{(\mathbf{a}_{x,x})^2+(\mathbf{a}_{y,y})^2+2\mathbf{a}_{x,x}\mathbf{a}_{y,y}\}+\frac{L}{2}(|\mathbf{a}|-\mathbf{a}_0)^2\\&+\frac{B}{2}(\mathbf{c}_{i,x}\mathbf{c}_{i,x}+\mathbf{c}_{i,y}\mathbf{c}_{i,y})-C(\mathbf{a}_{x,x}+\mathbf{a}_{y,y})(\mathbf{c}_{x,x}+\mathbf{c}_{y,y})\\&-\mathbf{P}_s(\mathbf{a}\times\mathbf{c})_y\mathbf{E}_y.\end{aligned} \tag{2a}$$

Then putting $\mathbf{a}(x,y,z)$ into $(-\phi_x, -\phi_y, 1)$ and $\mathbf{a}_0\simeq 1+(1/2)\theta_m^2$, we readily have

$$\begin{aligned}F=&\frac{A}{2}(\phi_{xx}^2+\phi_{yy}^2+2\phi_{xx}\phi_{yy})+\frac{L}{8}(\phi_x^2+\phi_y^2-\theta_m^2)^2\\&+\frac{B}{2}\{(\mathbf{c}_{x,x})^2+(\mathbf{c}_{x,y})^2+(\mathbf{c}_{y,x})^2+(\mathbf{c}_{y,y})^2+(\mathbf{c}_{z,x})^2+(\mathbf{c}_{z,y})^2\}\\&+C\{(\phi_{xx}+\phi_{yy})(\mathbf{c}_{x,x}+\mathbf{c}_{y,y})\}-\mathbf{P}_s\mathbf{E}(\mathbf{c}_x+\phi_x\mathbf{c}_z),\end{aligned} \tag{2b}$$

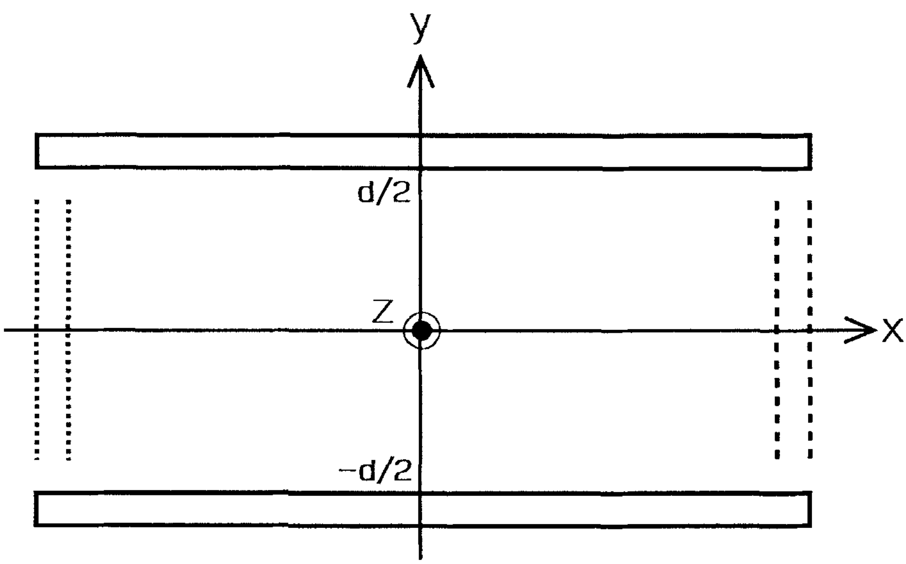


Figure 1. The coordinate system. Here d is the sample gap.

where ϕ is the layer deviation from a bookshelf layer structure as in the S_A phase and the following approximation was utilized:

$$(\phi_x^2+\phi_y^2+1)^{1/2} \simeq 1+\tfrac{1}{2}(\phi_x^2+\phi_y^2) \qquad (|\phi_x|,\ |\phi_y| \ll 1). \tag{3}$$

From the above free energy the Euler–Lagrange equations for ϕ can be derived as

$$\begin{aligned} &A(\phi_{xxxx}+\phi_{yyyy}+2\phi_{xxyy}) \\ &-\frac{L}{2}\{\phi_{xx}(3\phi_x^2+\phi_y^2-\theta_m^2)+\phi_{yy}(\phi_x^2+3\phi_y^2-\theta_m^2)+4\phi_{xy}\phi_x\phi_y\} \\ &+C(\mathbf{c}_{x,xxx}+\mathbf{c}_{y,yxx}+\mathbf{c}_{x,xyy}+\mathbf{c}_{y,yyy})+\mathbf{P}_s\mathbf{E}\mathbf{c}_{z,x} \\ &+(\mu_x\mathbf{c}_x+\mu\mathbf{c}_{x,x}+\mu_y\mathbf{c}_y+\mu\mathbf{c}_{y,y})=0. \end{aligned} \tag{4}$$

On the other hands the Euler–Lagrange equations for $\mathbf{c}_x$, $\mathbf{c}_y$ and $\mathbf{c}_z$ can be obtained as

$$v\mathbf{c}_x-\mu\phi_x-B(\mathbf{c}_{x,xx}+\mathbf{c}_{x,yy})-C(\phi_{xxx}+\phi_{yyx})-\mathbf{P}_s\mathbf{E}=0, \tag{5a}$$

$$v\mathbf{c}_y-\mu\phi_y-B(\mathbf{c}_{y,xx}+\mathbf{c}_{y,yy})-C(\phi_{xxy}+\phi_{yyy})=0, \tag{5b}$$

$$v\mathbf{c}_z+\mu-B(\mathbf{c}_{z,xx}+\mathbf{c}_{z,yy})-\mathbf{P}_s\mathbf{E}\phi_x=0, \tag{5c}$$

where μ and v are the Lagrange multipliers introduced to satisfy $\mathbf{a}\cdot\mathbf{c}=0$ as well as $\mathbf{c}\cdot\mathbf{c}=1$, respectively. In the following, however, we shall assume a weak distortion such that $\mathbf{a}\cdot\mathbf{c}\simeq 0$ or $\mu\simeq 0$, and that $\mathbf{c}\cdot\mathbf{c}\simeq 1$ with $\mathbf{c}_x\simeq 1$ or $v\simeq 0$, for simplicity and from equations (5 *a*), (5 *b*) and (5 *c*), we obtain the following:

$$(\mathbf{c}_{x,xx}+\mathbf{c}_{x,yy})=-(C/B)(\phi_{xxx}+\phi_{yyx})-\mathbf{e}, \tag{6a}$$

$$(\mathbf{c}_{y,xx}+\mathbf{c}_{y,yy})=-(C/B)(\phi_{xxy}+\phi_{yyy}), \tag{6b}$$

$$(\mathbf{c}_{z,xx}+\mathbf{c}_{z,yy})=-\mathbf{e}\phi_x, \tag{6c}$$

where $\mathbf{e}$ is a normalized electric field and defined by

$$\mathbf{e}=\frac{\mathbf{P}_s\mathbf{E}}{B}. \tag{7}$$

From equations (6 *a*) and (6 *b*) we have

$$(\mathbf{c}_{x,xxx}+\mathbf{c}_{y,yxx}+\mathbf{c}_{x,xyy}+\mathbf{c}_{y,yyy})=-\frac{C}{B}(\phi_{xxxx}+2\phi_{xxyy}+\phi_{yyyy}). \tag{8}$$

Substituting equation (8) into equation (4) and eliminating $\mathbf{c}_x$ and $\mathbf{c}_y$, we find

$$\begin{aligned} &\left(A-\frac{C^2}{B}\right)\cdot(\phi_{xxxx}+\phi_{yyyy}+2\phi_{xxyy}) \\ &-\frac{L}{2}\{\phi_{xx}(3\phi_x^2+\phi_y^2-\theta_m^2)+\phi_{yy}(\phi_x^2+3\phi_y^2-\theta_m^2)+4\phi_{xy}\phi_x\phi_y\} \\ &+\mathbf{P}_s\mathbf{E}\mathbf{c}_{z,x}=0. \end{aligned} \tag{9}$$

Normalizing ϕ, x, and y by λ and denoting them as ψ, ξ and η, respectively, we have

$$\begin{aligned} &\{\psi_{\xi\xi\xi\xi}+\psi_{\eta\eta\eta\eta}+2\psi_{\xi\xi\eta\eta}\} \\ &\quad=\tfrac{1}{2}[\psi_{\xi\xi}(3\psi_\xi^2+\psi_\eta^2-\theta_m^2)+\psi_{\eta\eta}(\psi_\xi^2+3\psi_\eta^2-\theta_m^2)+4\psi_{\xi\eta}\psi_\xi\psi_\eta] \\ &\quad-\mathbf{e}\left(\frac{B}{L}\right)\mathbf{c}_{z,\xi}, \end{aligned} \tag{10}$$

where λ is defined by

$$\frac{1}{\lambda^2}=\frac{L}{A-(C^2/B)}. \tag{11}$$

Next, denoting the division length for ξ and η axes as h^*, we have the following set of equations corresponding to equation (10) as

$$\begin{aligned}
&\psi_{i+2,j}-8\psi_{i+1,j}+20\psi_{i,j}-8\psi_{i-1,j}+\psi_{i-2,j}+\psi_{i,j+2}\\
&\quad-8\psi_{i,j+1}-8\psi_{i,j-1}+\psi_{i,j-2}+2\psi_{i+1,j+1}-2\psi_{i+1,j-1}\\
&\quad+2\psi_{i-1,j+1}+2\psi_{i-1,j-1}\\
&=\frac{1}{2}\left[\begin{array}{l}(\psi_{i+1,j}-2\psi_{i,j}+\psi_{i-1,j})\cdot\{3(f_1)^2+(f_2)^2-\theta_{\mathrm{m}}^2h^{*2}\}\\ +(\psi_{i,j+1}-2\psi_{i,j}+\psi_{i,j-1})\cdot\{(f_1)^2+3(f_2)^2-\theta_{\mathrm{m}}^2h^{*2}\}\\ +(\psi_{i+1,j+1}-\psi_{i+1,j-1}-\psi_{i-1,j+1}+\psi_{i-1,j-1})\cdot(f_3)\\ -(\mathbf{c}_{zi,j+1}-\mathbf{c}_{zi,j-1})h^{*3}\cdot\mathbf{e}\cdot(B/L)\}\end{array}\right],
\end{aligned} \tag{12}$$

where f_1, f_2 and f_3 are defined as

$$f_1=(\psi_{i+1,j}-\psi_{i-1,j})/2, \tag{13a}$$

$$f_2=(\psi_{i,j+1}-\psi_{i,j-1})/2, \tag{13b}$$

$$f_3=f_1f_2=(\psi_{i+1,j}-\psi_{i-1,j})(\psi_{i,j+1}-\psi_{i,j-1})/4. \tag{13c}$$

Next, from equations (6 *a*), (6 *b*) and (6 *c*), we obtain the differential equations for the $\mathbf{c}$ director

$$\mathbf{c}_{x,\xi\xi}+\mathbf{c}_{x,\eta\eta}=-(C/B)(\psi_{\xi\xi\xi}+\psi_{\eta\eta\xi})-\lambda^2\mathbf{e}, \tag{14a}$$

$$\mathbf{c}_{y,\xi\xi}+\mathbf{c}_{y,\eta\eta}=-(C/B)(\psi_{\xi\xi\eta}+\psi_{\eta\eta\eta}), \tag{14b}$$

$$\mathbf{c}_{z,\xi\xi}+\mathbf{c}_{z,\eta\eta}=-\lambda^2\mathbf{e}\psi_{\xi}. \tag{14c}$$

Then, normalizing in the same way, we have

$$\begin{aligned}
\mathbf{c}_{xi,j}=&\frac{C}{8Bh^*}(\psi_{i+2,j}-4\psi_{i+1,j}+4\psi_{i-1,j}-\psi_{i-2,j}\\
&+\psi_{i+1,j+1}+\psi_{i+1,j-1}-\psi_{i-1,j+1}-\psi_{i-1,j-1})\\
&+(1/4)\{\mathbf{c}_{xi+1,j}+\mathbf{c}_{xi-1,j}+\mathbf{c}_{xi,j+1}+\mathbf{c}_{xi,j-1}\}+\frac{\mathbf{e}h^{*2}\lambda^2}{4},
\end{aligned} \tag{15}$$

$$\begin{aligned}
\mathbf{c}_{yi,j}=&\frac{C}{8Bh^*}(\psi_{i,j+2}-4\psi_{i,j+1}+4\psi_{i,j-1}-\psi_{i,j-2}\\
&+\psi_{i+1,j+1}+\psi_{i-1,j+1}-\psi_{i+1,j-1}-\psi_{i-1,j-1})\\
&+(1/4)\{\mathbf{c}_{yi+1,j}+\mathbf{c}_{yi-1,j}+\mathbf{c}_{yi,j+1}+\mathbf{c}_{yi,j-1}\},
\end{aligned} \tag{16}$$

$$\begin{aligned}
\mathbf{c}_{zi,j}=&(1/4)\{\mathbf{c}_{zi+1,j}+\mathbf{c}_{zi-1,j}+\mathbf{c}_{zi,j+1}+\mathbf{c}_{zi,j-1}\}\\
&+\frac{\mathbf{e}h^*\lambda^2}{8}\{\psi_{i+1,j}-\psi_{i-1,j}\}.
\end{aligned} \tag{17}$$

From equations (13), (15)–(17), we can analyse the layer structure under an electric field.

3. Numerical results

In this section, we present some numerical results for the analysis of the two dimensional layer structure in the S_C^* phase and we put the parameters λ, C/B, B/L to 1 through the following numerical results.

We suppose now the following boundary conditions for ψ:

$$\psi(-w^*/2,\eta)=2\log\left(\frac{\cosh(\theta_m d^*/4)}{\cosh(\theta_m\eta/2)}\right)>0 \quad \text{for } \xi=-w^*/2, \qquad (18\,a)$$

$$\psi(+w^*/2,\eta)=-2\log\left(\frac{\cosh(\theta_m d^*/4)}{\cosh(\theta_m\eta/2)}\right)<0 \quad \text{for } \xi=+w^*/2, \qquad (18\,b)$$

where w^* is assumed to be the normalized thickness of the domain boundary and d^* is defined as (the cell gap)/λ. In the following results we put $w^*=2d^*$. The boundary condition for the **c** director is given by

$$\mathbf{c}(\xi, +d^*/2)=(\pm 1,0,0), \qquad (19\,a)$$

$$\mathbf{c}(\xi, -d^*/2)=(\pm 1,0,0). \qquad (19\,b)$$

First we show the dependence of the layer structure on the molecular tilt angle θ_m in figures 2 (*a*) and (*b*). From these results we can see that the chevron structure becomes more appreciable by increasing the molecular tilt angle, which is consistent with experimental findings [1].

In figures 3 (*a*) and (*b*) we show the effect of the sample thickness d^*. In this case, it is found that the chevron structure becomes apparently more appreciable by increasing the sample thickness.

Finally the electric field effects are presented in figures 4 (*a*) and (*b*). From these results, we see that the electric field $\mathbf{e}>0$ orients the **c** director towards the $+\xi$ direction or the spontaneous polarization towards the $+\eta$ direction. On the contrary, for $\mathbf{e}<0$, the **c** director aligns along the $-\xi$ direction, or the spontaneous polarization along the $-\eta$ direction as shown in figures 5 (*a*) and (*b*).

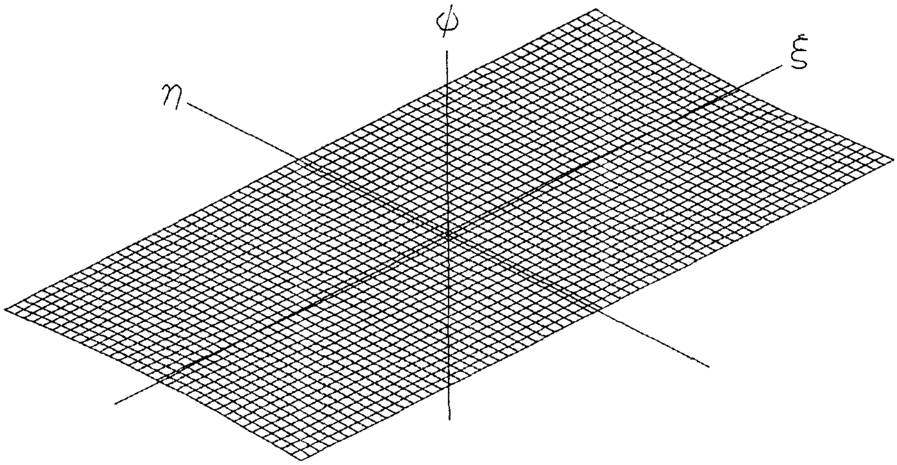
4. Concluding remarks

In the present work, we have analysed the layer structure in the boundary region between two chevrons with opposite directions. From the numerical results, the following was found:

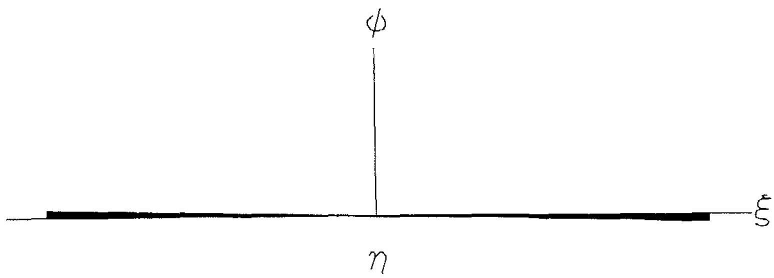
(i) The chevron layer structure becomes more like a kink-solution by increasing the molecular tilt and the sample gap.

(ii) The chevron structure can be considerably distorted, with an undulation along the η axis, under an external electric field as can be seen from figures 4 (*a*2) and (*b*2). The **c** director is then oriented along the ξ axis with the spontaneous polarization along the η axis.

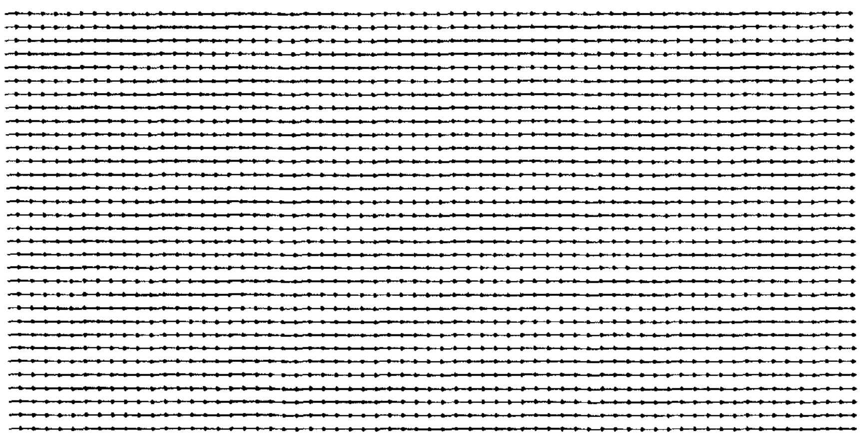
In the present analysis, although we assumed a weak distortion with $\mu\simeq 0$ and $\nu\simeq 0$ for simplicity, it seems to be important to take it more into account under a relatively strong distortion. The analysis of such a condition is now in progress and will be reported in the near future together with a comparison with some experimental observations [2].



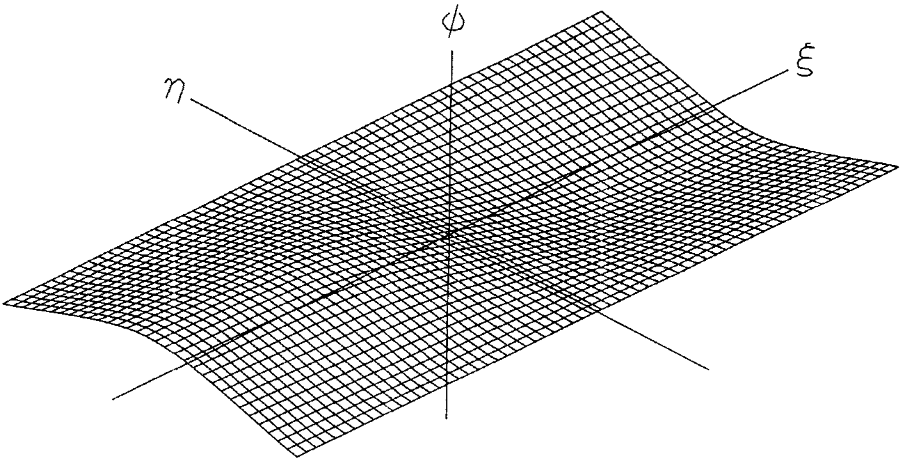
(*a*1)



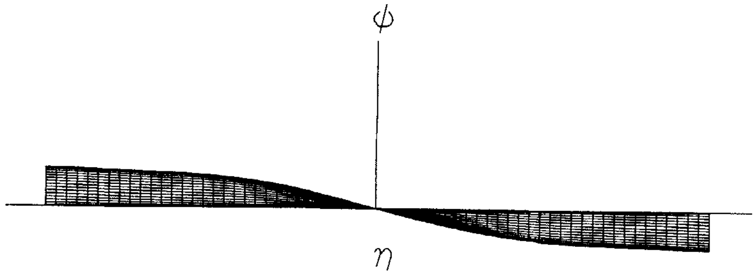
(*a*2)



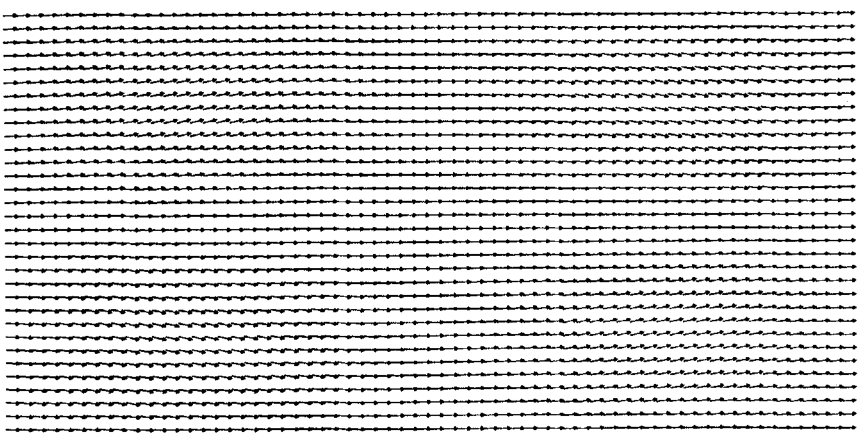
(*a*3)



(*b*1)

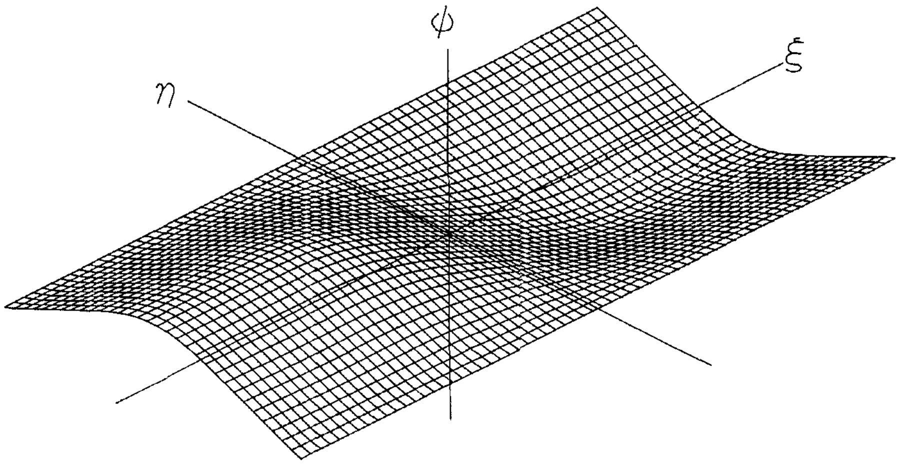


(*b*2)

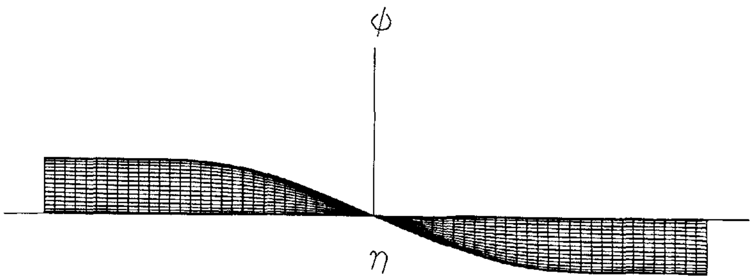


(*b*3)

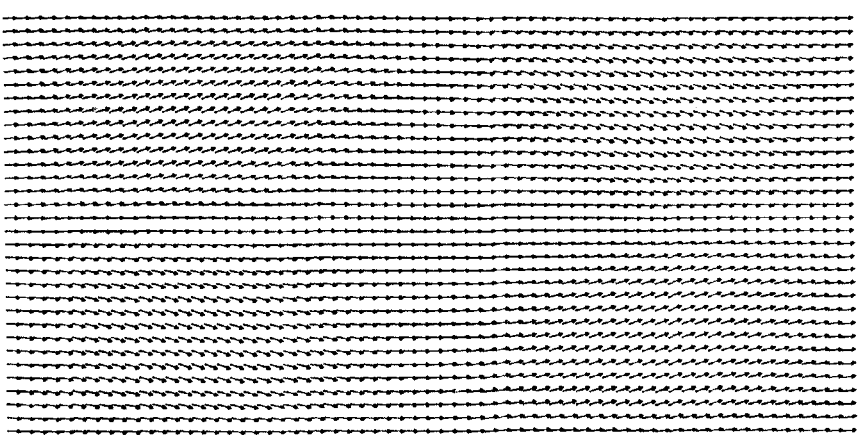
Figure 2. The effect of the molecular tilt angle θ_m. Here $d^* = 40$ and $\mathbf{e} = 0$. (*a*) $\theta_m = 0{\cdot}1$. (*a*1) and (*a*2) the layer structure. (*a*3) The **c** director configuration. (*b*) $\theta_m = 0{\cdot}3$. (*b*1) and (*b*2) the layer structure. (*b*3) The **c** director configuration.



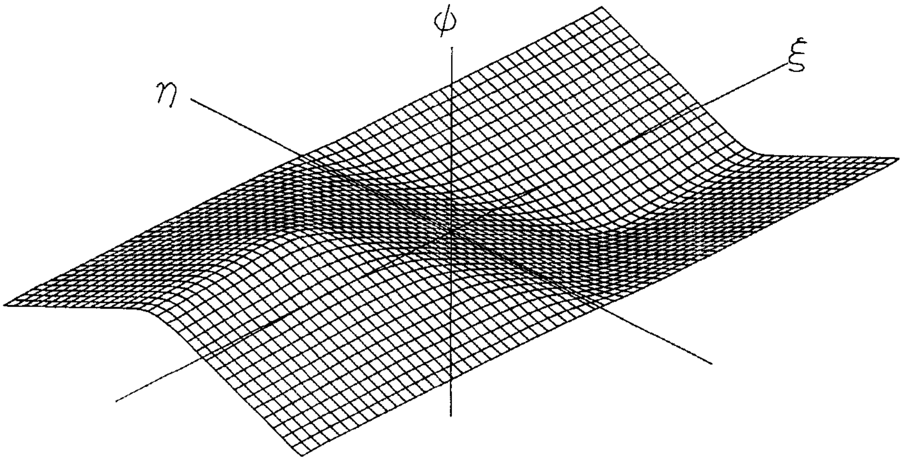
(a1)



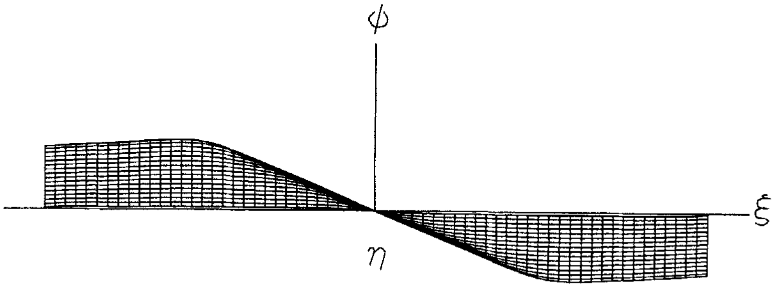
(a2)



(a3)



(b1)



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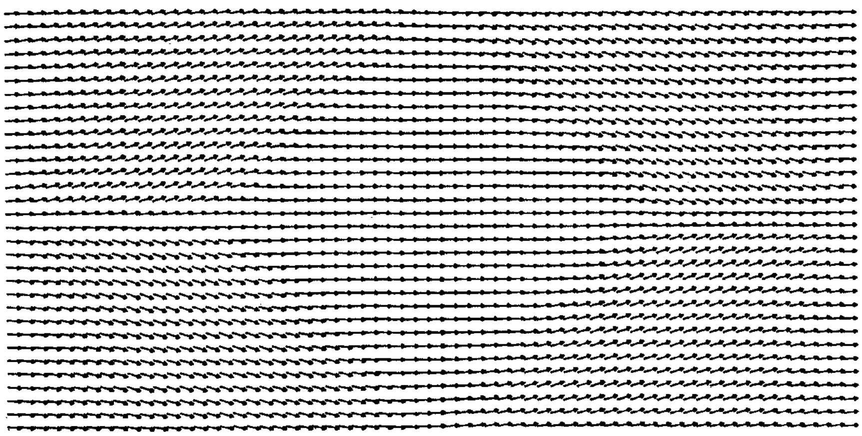
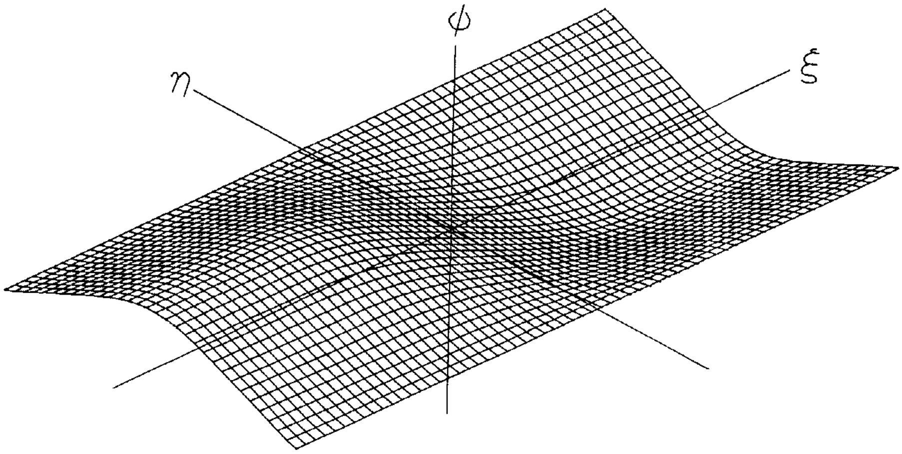
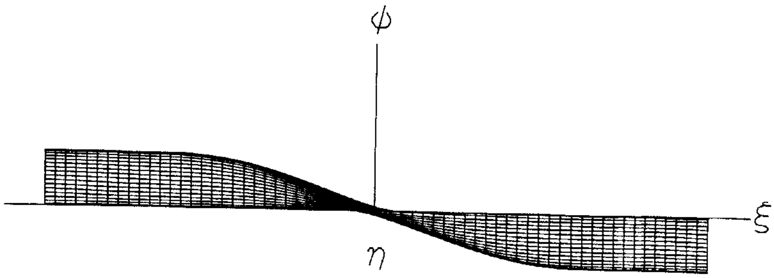


(b3)

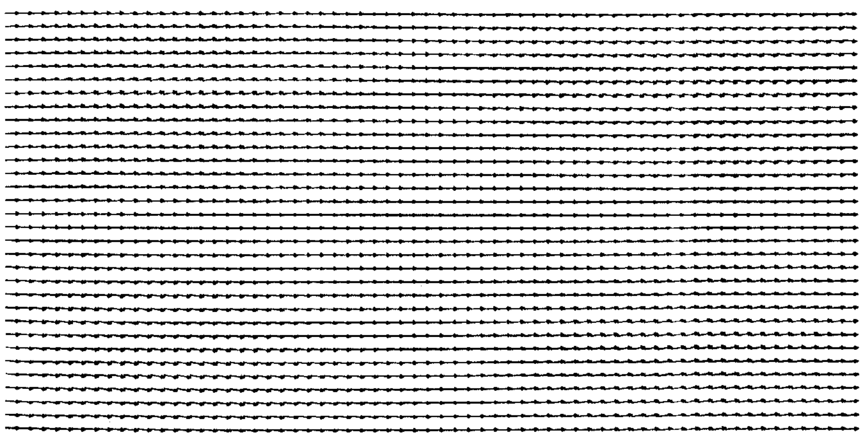
Figure 3. The effect of the sample gap. Here $\theta_m = 0{\cdot}4$ and $\mathbf{e} = 0$. (a) $d^* = 40$. (a1) and (a2) the layer structure. (a3) The **c** director configuration. (b) $d^* = 100$. (b1) and (b2) the layer structure. (b3) The **c** director configuration.



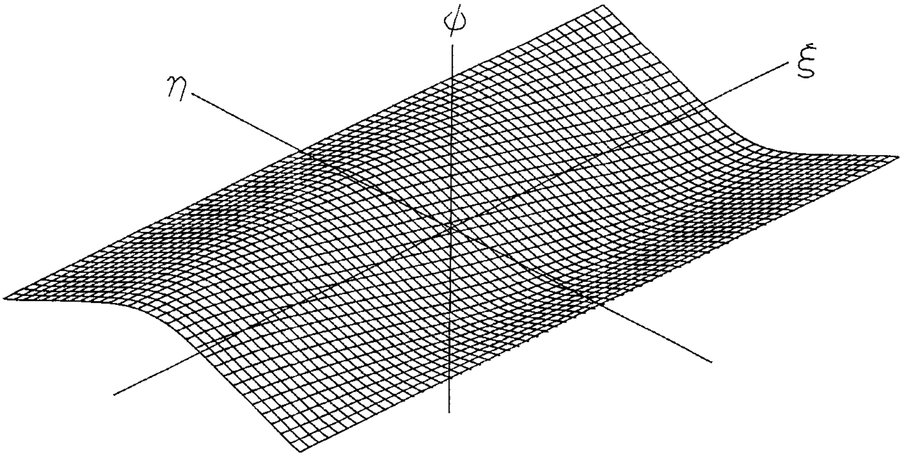
(a1)



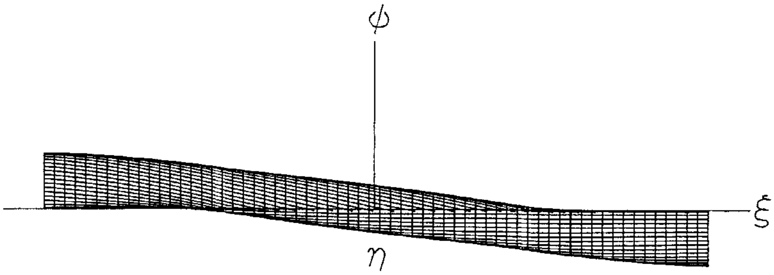
(a2)



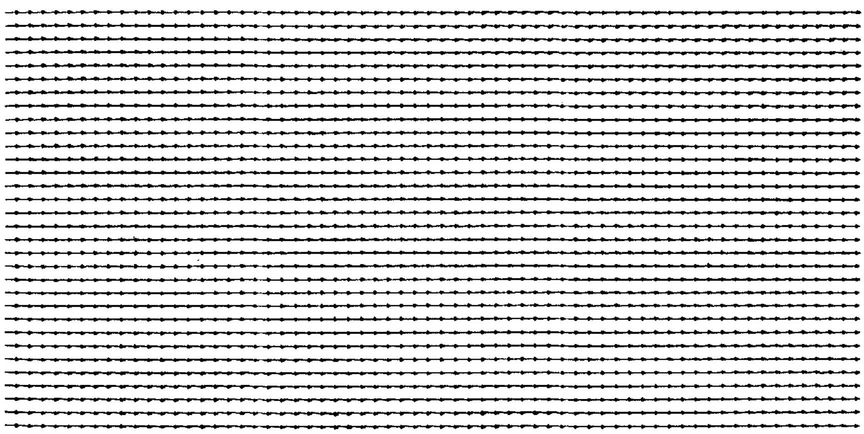
(a3)



(b1)

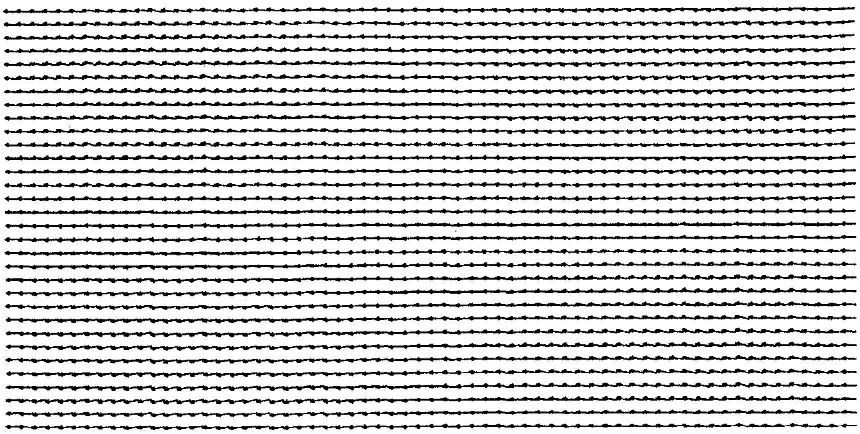


(b2)

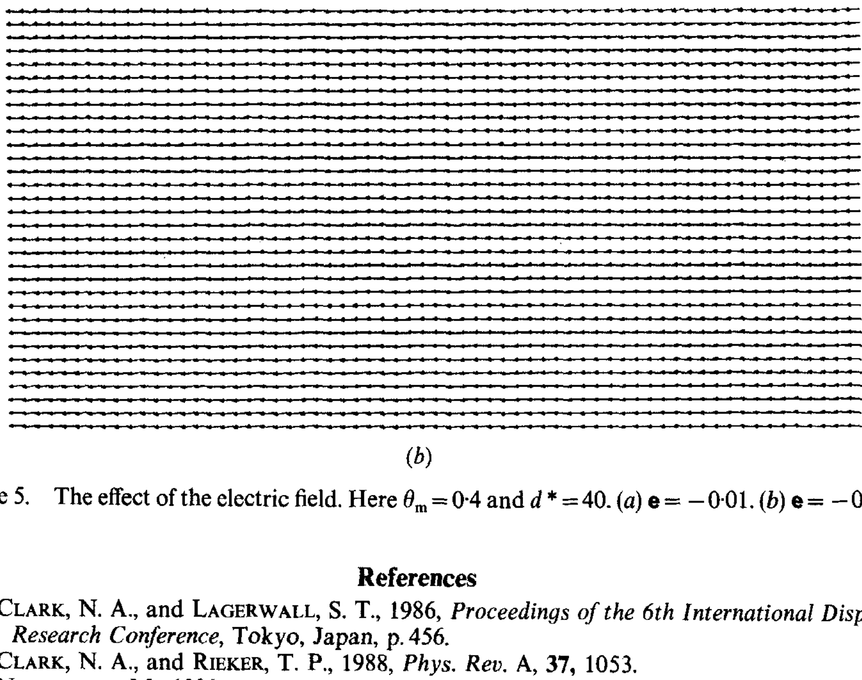


(b3)

Figure 4. The effect of the electric field. Here $\theta_m = 0{\cdot}4$ and $d^* = 40$. (a) $\mathbf{e} = 0{\cdot}01$. (a1) and (a2) the layer structure. (a3) The $\mathbf{c}$ director configuration. (b) $\mathbf{e} = 0{\cdot}03$. (b1) and (b2) the layer structure. (b3) The $\mathbf{c}$ director configuration.



(*a*)



(*b*)

Figure 5. The effect of the electric field. Here $\theta_m = 0{\cdot}4$ and $d^* = 40$. (*a*) $\mathbf{e} = -0{\cdot}01$. (*b*) $\mathbf{e} = -0{\cdot}03$.

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