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ORIENTATIONAL STRUCTURES IN CHIRAL NEMATIC LIQUID CRYSTALS FOR WEAK ANCHORING

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ABSTRACT **This work presents a unitary mode to describe orientational structures of extreme free energy for unidimensional distortions of a chiral nematic layer with weak tilted anchoring at limiting surfaces, using structure parameters. The case of an applied electric field was also considered. A generalised expression for surface energy involving both polar and azimuthal deformations was introduced. A classification of possible structures having monotonous or non-monotonous variations of the tilt angle is presented. The solving of the equation system that links the structure parameters in each case is given.**

INTRODUCTION

In the last decades many papers were devoted to the study of orientational structures appearing in cells with nematic liquid crystals (more general chiral nematics or cholesteric liquid crystals with large pitch), bounded by solid surfaces having orientational properties on the liquid crystal, in the absence or presence of external fields. Generally speaking, simple structures characterised by symmetry or anti-symmetry from the middle of the cell of molecular orientation distortion in bulk, due to the symmetry or anti-symmetry of the anchoring conditions at the boundaries of the cells, were studied.[1,2] The use of simple orientational geometries produced by tangential or normal surface molecular anchoring at the boundary surfaces, allowed to obtain methods for determination of material constants (e.g. elastic constants[3]) or anchoring strength at the surface.[4] These geometries are characterised by the existence of

threshold fields to which the constants are directly linked, and their theoretical treatment involves a restraint number of equations. Moreover, the using of simplifying hypothesises led, often, to some analytical approximate results.[5,6] However, the development of liquid crystals displays imposed the use of oblique surface anchoring conditions at the boundary surfaces and/or the doping of the nematic with chiral materials, giving it cholesteric liquid crystal properties. All these resulted as a necessity to eliminate some non-uniformities of the aspect[7] or as an essential condition for the given phenomenon to appear.[8,9,10] Nowadays, there are techniques of obtaining layers with properties of surface alignment of liquid crystal which allow to obtain controlled tilt angles in the whole domain from 0 to 90°.[11,12,13] Such layers cannot be, generally, characterised by strong anchoring. In addition, it cannot be considered that the two limiting surfaces of the cell assure identical anchoring conditions (from the tilt or strength point of view).

The general case cannot be any longer solved using a single equation, nor to be reduced to analytical forms, the only solution after writing the corresponding equations being a numerical one. Treatments of the equilibrium structure problem for (chiral) nematic, under conditions of strong and tilted anchoring[14,15] show that the different possible structures can be characterised, in bulk, by the existence of maxima or minima of the tilt angle, or by monotonous variations (the absence of extremes). In addition, for symmetrical anchoring, the extremum of tilt angle is placed in the middle of the cell. Although a description using extreme tilt angles is very suggestive and useful in interpreting some structures (and their calculation), using such structure parameters for characterisation of the structure isn't generally suitable.

The aim of this work is to present a way to describe bulk and surface free energy extreme structures for the general case of a cholesteric liquid crystal layer, subject to an electric field, in the case of weak, tilted, different at the two boundary surfaces anchoring.

HYPOTHESIS AND NOTATIONS

Liquid crystal

Let us consider a chiral nematic liquid crystal characterised by the pitch P, the elastic constants K_{11}, K_{22}, K_{33} and the dielectric ones $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$.

The cell

The liquid crystal is confined between two plan parallel surfaces situated at $z=0$ and

z=L and having orientational properties on the liquid crystal molecules. The boundary surfaces play also the role of electrodes on which a constant electric voltage can be applied.

The orientation of the liquid crystal

The molecular orientation everywhere in the liquid crystal layer, including the boundary surfaces is given by the director versor $\vec{n}$, specified by the tilt angle α and the azimuthal angle β, so that:

$$\vec{n}=\vec{n}\ (\alpha,\beta)=(\cos\alpha\cdot\cos\beta,\cos\alpha\cdot\sin\beta,\sin\alpha) \qquad (1)$$

Easy directions on the surfaces

We suppose that the two surfaces have been treated in such a way so that each has a uniform molecular easy direction. Let be the easy direction of alignment $\vec{n}_0(\alpha_0,\beta_0)$ at z=0 given by the tilt angle $\alpha_0>0$ and the azimuthal angle $\beta_0=0$. At the other boundary surface z=L the easy direction of alignment $\vec{n}_1(\alpha_1,\beta_1)$ is given by a tilt angle $\alpha_1\neq\alpha_0$ and an azimuthal mounting angle $-\pi<\beta_1<\pi$.

Surface anchoring

Let be a limiting surface S, characterised by an easy direction given by the versor $\vec{n}_S=\vec{n}(\alpha_S,\beta_S)$. For weak anchoring, the liquid crystal can achieve on the limiting surface an orientation $\vec{n}(S)=\vec{n}(\alpha(S),\beta(S))$, different from $\vec{n}_S$ by the tilt, as well as by the azimuthal angles. For this, we consider a form of the density of the surface energy that is a generalisation of the form given by Rapini and Papoular[16], $W_S=1/2\cdot W_0\sin^2(\alpha(S)-\alpha_S)$, which takes into account only the deviation of tilt angle. W_0 is the anchoring strength. We will consider at the orientational surface besides the easy direction $\vec{n}_S$, another two perpendicular on it directions and linked to it and to $\vec{k}$, the normal at the surface:

- the first direction $\vec{n}_{ST}\sim\vec{k}\times\vec{n}_S$ is situated in the plane of surface and mainly describes a twist surface distortion with regard to the easy direction,

- the second direction $\vec{n}_{SH}\sim\vec{n}_S\times\vec{n}_{ST}$ is situated in the plane determined by the easy direction and the normal to the surface and describes a tilt surface distortion.

The anchoring energy of the unit area, that is minimum when $\vec{n}(S)$ is parallel to $\vec{n}_S$, can be generally written as the sum of two contributions:

$$W_S(\vec{n}_S,\vec{n}(S))=\frac{1}{2}W_H\cdot(\vec{n}_{SH}\cdot\vec{n}(S))^2+\frac{1}{2}W_T\cdot(\vec{n}_{ST}\cdot\vec{n}(S))^2 \quad \text{or}$$

$$W_S(\vec{n}_S, \vec{n}(S)) = \frac{1}{2}W_H\left[\sin\alpha(S)\cos\alpha_S - \cos\alpha(S)\cos(\beta(S)-\beta_S)\sin\alpha_S\right]^2 + \\ + \frac{1}{2}W_T \cdot \cos^2\alpha(S)\sin^2(\beta(S)-\beta_S) \quad (2)$$

where W_T and W_H are the anchoring strengths for the two types of surface deformations and are responsible for the anisotropy of anchoring strength. In the particular case when $W_T=W_H$, the surface energy depends only on the angle between $\vec{n}(S)$ and $\vec{n}_S$, $W_S = \frac{1}{2}W_H\left\{1-\left[\vec{n}_S \cdot \vec{n}(S)\right]^2\right\}$, form that is of an already proposed type.[2,17]

The hypothesis of unidimensional distortion

We suppose that the molecular orientation in every plane z=constant in the liquid crystal bulk doesn't depend on x and y so that $\alpha=\alpha(z)$ and $\beta=\beta(z)$. Also all variables that characterise the system depend only on z, and their derivatives in function of x or y are zero.

In the case of a constant electric voltage applied to the system, the thermodynamic equilibrium will corresponds to the minimum of the free energy Gibbs G.[18] This energy contains bulk (elastic and electric) and surface contributions:

$$G = \text{Area} \cdot \left\{\int_0^L (w_k - w_e)dz + W_S\left[\vec{n}_0, \vec{n}(0)\right] + W_S\left[\vec{n}_L, \vec{n}(L)\right]\right\} \quad (3)$$

$w_e = \frac{1}{2}\vec{E}\cdot\vec{D}$ is the bulk density of the electric field in the liquid crystal layer.

The unidimensional distortion hypothesis for an insulator under a constant voltage leads to $\frac{\partial D_z}{\partial z} = 0$, i.e. D_z is independent on z, but functionally depends on the orientational configuration (D_z plays the role of a structural parameter).

$$\frac{G}{Area}=\int_0^L\left(w_k+\frac{1}{2}\cdot\frac{D_z^2}{\varepsilon_{||}\sin^2\alpha+\varepsilon_\perp\cos^2\alpha}\right)dz+W_{S0}+W_{SL}=\frac{K_{11}}{2L}\int_0^1 w_{bulk}d\xi+W_S$$

where D_z has to be considered as a true constant.

We introduced w_{bulk} to express the integral in an adimensionalised form:

$$w_{bulk}(\alpha,\dot\alpha,\beta)=(1+a\cdot\sin^2\alpha)\dot\alpha^2+c\cdot\dot\beta\cdot\left[\dot\beta\cdot(1+b\cdot\sin^2\alpha)\cos^2\alpha-2\cdot Q\cdot\cos^2\alpha\right]+\frac{D^2}{d}\cdot\frac{S(d)}{1+d\cdot\sin^2\alpha} \qquad (5)$$

where we used :

$$\left.\begin{aligned}&\xi=\frac{z}{L},\quad \dot\alpha=\frac{\partial\alpha}{\partial\xi},\quad \dot\beta=\frac{\partial\beta}{\partial\xi},\quad S(\eta)=\begin{cases}-1 & \eta<0\\ 0 & \eta=0\\ 1 & \eta>0\end{cases}\\ &a=\frac{K_{33}-K_{11}}{K_{11}},\ b=\frac{K_{33}-K_{22}}{K_{22}},\ c=\frac{K_{22}}{K_{11}},\ d=\frac{\varepsilon_{||}-\varepsilon_\perp}{\varepsilon_\perp},\\ &Q=q\cdot L=\frac{2\pi L}{P},\ D=\frac{D_zL/\varepsilon_\perp}{U_0},\ \text{where}\ U_0=\sqrt{\frac{K_{11}}{|\varepsilon_{||}-\varepsilon_\perp|}}\end{aligned}\right\} \qquad (6)$$

In the above notations there are two adimensional structural parameters, D and Q, the first replacing the parameter D_z and the latter, the thickness L.

The bulk equilibrium equations are:

$$0=\frac{\partial w_{bulk}}{\partial\beta}=\frac{d}{d\xi}\left(\frac{\partial w_{bulk}}{\partial\dot\beta}\right) \qquad (7.1)$$

$$\frac{\partial w_{bulk}}{\partial\alpha}=\frac{d}{d\xi}\left(\frac{\partial w_{bulk}}{\partial\dot\alpha}\right) \qquad (7.2)$$

After a first integration, these eqs. become:

$$\dot\beta=\frac{B+Q\cdot\cos^2\alpha}{(1+b\cdot\sin^2\alpha)\cos^2\alpha} \qquad (8.1)$$

$$\dot\alpha^2=\frac{\dfrac{D^2}{d}\cdot\dfrac{S(d)}{1+d\cdot\sin^2\alpha}-c\cdot\dfrac{(B+Q\cdot\cos^2\alpha)^2}{(1+b\cdot\sin^2\alpha)\cos^2\alpha}+A}{1+a\cdot\sin^2\alpha}=f(\alpha,A,B,D,Q) \qquad (8.2)$$

where A and B are integration constants and play the role of structural parameters as well as D and Q.

The equilibrium equations, due to the surfaces, can be written as:

$$\frac{2\pi K_{11}}{QP}\cdot\dot{\alpha}(0)\left(1+a\cdot\sin^2\alpha(0)\right)=\frac{\partial W_S}{\partial\alpha(0)} \tag{8.3}$$

$$\frac{2\pi K_{11}}{QP}\cdot c\cdot B=\frac{\partial W_S}{\partial\beta(0)} \tag{8.4}$$

$$-\frac{2\pi K_{11}}{QP}\cdot\dot{\alpha}(1)\left(1+a\cdot\sin^2\alpha(1)\right)=\frac{\partial W_S}{\partial\alpha(1)} \tag{8.5}$$

$$-\frac{2\pi K_{11}}{QP}\cdot c\cdot B=\frac{\partial W_S}{\partial\beta(1)} \tag{8.6}$$

Possible solution types

An extreme free energy structure of the liquid crystal system in an electric field is characterised by a set of 8 structural parameters $\mathfrak{R}=\mathfrak{R}[A,B,D,Q,\alpha(0),\beta(0),\alpha(1),\beta(1)]$ that is a solution of the equation system (8). From the condition $f(\alpha,A,B,D,Q)\geq 0$ the equation (8.2) gives a necessary condition for the validity of the set of parameters $\mathfrak{R}$. In the same time it gives qualitative information about allowed variation mode of molecular tilt angle, from one surface to the other. The tilt angle α, for which $f(\alpha,A,B,D,Q)=0$ may play the role of an extreme tilt angle for the orientational structure because in this case, $d\alpha/d\xi=0$.

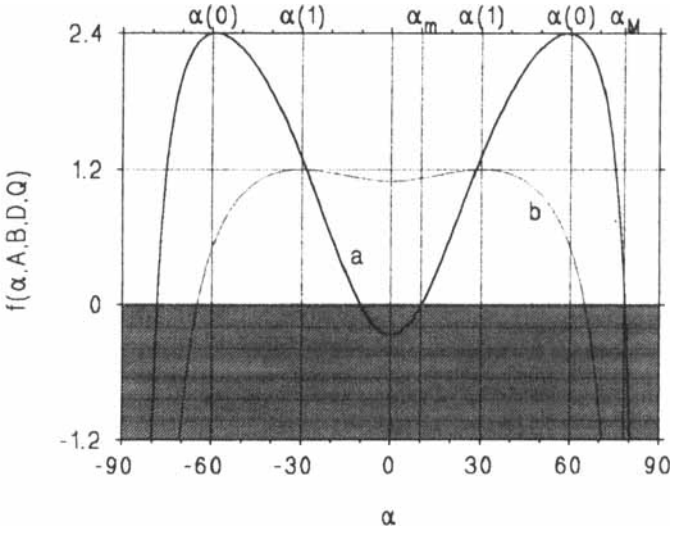

FIGURE 1 Two examples of variation of function $f(\alpha,A,B,D,Q)$, given by equation (8.2) vs. the tilt angle α.

TABLE I Labels and description of orientational structures

Type	Mode of variation of the tilt angle	N	Integration path	$\sigma(S)$
5	$\alpha(0)\nearrow\alpha_M\searrow\alpha(0)\searrow-\alpha_M\nearrow\alpha(1)$	2	$\Theta(0)\to\pi/2\to\pi-\Theta(0)$ followed by $\pi-\Theta(0)\to3\pi/2\to2\pi+\Theta(1)$	$\sigma(0)=1$ $\sigma(1)=1$
4	$\alpha(0)\searrow\alpha_m\nearrow\alpha(0)\nearrow\alpha_M\searrow\alpha(1)$	2	$-\theta(0)\to0\to\theta(0)$ followed by $\Theta(0)\to\pi/2\to\pi-\Theta(1)$	$\sigma(0)=-1$ $\sigma(1)=-1$
3	$\alpha(0)\nearrow\alpha_M\searrow\alpha(0)\searrow\alpha_m\nearrow\alpha(1)$	2	$\Theta(0)\to\pi/2\to\pi-\Theta(0)$ followed by $-\theta(0)\to0\to\theta(1)$	$\sigma(0)=1$ $\sigma(1)=1$
2	$\alpha(0)\searrow\alpha_m\nearrow\alpha(1)$	1	$-\theta(0)\to0\to\theta(1)$	$\sigma(0)=-1$ $\sigma(1)=1$
1	$\alpha(0)\nearrow\alpha_M\searrow\alpha(1)$	1	$\Theta(0)\to\pi/2\to\pi-\Theta(1)$	$\sigma(0)=1$ $\sigma(1)=-1$
0	Monotonous variation	1	$\alpha(0)\to\alpha(1)$	*)
-1	$\alpha(0)\searrow-\alpha_M\nearrow\alpha(1)$	1	$\pi-\Theta(0)\to3\pi/2\to2\pi+\Theta(1)$	$\sigma(0)=-1$ $\sigma(1)=1$
-2	$0>\alpha(0)\nearrow-\alpha_m\searrow\alpha(1)<0$	1	$\pi-\theta(0)\to\pi\to\pi+\theta(1)$	$\sigma(0)=1$ $\sigma(1)=-1$
-3	$0>\alpha(0)\searrow-\alpha_M\nearrow\alpha(0)\nearrow-\alpha_m\searrow\alpha(1)<0$	2	$\pi-\Theta(0)\to3\pi/2\to2\pi+\Theta(0)$ followed by $\pi-\theta(0)\to\pi\to\pi+\theta(1)$	$\sigma(0)=-1$ $\sigma(1)=-1$
-4	$0>\alpha(0)\nearrow-\alpha_m\searrow\alpha(0)\searrow-\alpha_M\nearrow\alpha(1)<0$	2	$\pi-\theta(0)\to\pi\to\pi+\theta(0)$ followed by $\pi-\Theta(0)\to3\pi/2\to2\pi+\Theta(1)$	$\sigma(0)=1$ $\sigma(1)=1$
-5	$\alpha(0)\searrow-\alpha_M\nearrow\alpha(0)\nearrow\alpha_M\searrow\alpha(1)$	2	$\pi-\Theta(0)\to3\pi/2\to2\pi+\Theta(0)$ followed by $\Theta(0)\to\pi/2\to\pi-\Theta(1)$	$\sigma(0)=-1$ $\sigma(1)=-1$

*) $\sigma(0)=S[\alpha(1)-\alpha(0)]$, $\sigma(1)=-\sigma(0)$,

N is the number of intervals for integration in eqs. (9-11),

$\sigma(S)$ is the sign of the tilt angle variation near the surfaces 0 or 1,

$\Theta(S)$ is defined in APPENDIX A,

$\theta(S)$ is defined in APPENDIX B.

In figure 1 two examples of variations of the function $f(\alpha,A,B,D,Q)$ for two sets of structural parameters A, B, D and Q supposes to be parameters of extremum free energy structures are given. We considered as potentially valid all the tilt angles between -90° and +90°, in bulk as well as on the surfaces. As it can be remarked, the function is symmetrical. It may have an even number of roots. We note by α_M the root with the highest absolute value (which always exists) respectively by α_m, the modulus of the nearest root to $\alpha=0$ (when this exists, as in the case for the curve a).

Let us consider the example represented by the curve a from figure 1 for which $\alpha_M=78°$ and $\alpha_m=10°$. In function of the surface tilt angle values one can distinguish the following situations:

a) If one of the anchoring angles at the surfaces is positive and the other, negative, then on the account that the function $f(\alpha,A,B,D,Q)$ takes negative values in the inner interval from $\alpha(0)$ to $\alpha(1)$, the set of parameters $\Re$, which produced the function, are not able to represent a valid set of structural parameters.

b) If the anchoring angles $\alpha(0)$ and $\alpha(1)$ are both positive in the interval $[\alpha_m,\alpha_M]$, or both negative in the interval $[-\alpha_M,-\alpha_m]$, five types of structures/solutions for the parameters $\Re$ are possible. In the first case the solutions labelled by 0, 1, 2, or 4 in TABLE I are possible. In the second case, those labelled by 0, -1, -2, -3 or -4.

In the example represented by the curve b in Figure 1, for the anchoring angles $\alpha(0)$ and $\alpha(1)$ with values in the interval $[-\alpha_M,\alpha_M]$, five type of structures/solutions, namely those labelled by 0, ±1 or ±5 can also exist.

In each case five solutions, with different variation modes of the tilt angle between the surfaces can exist: monotonous variation: case 0; non-monotonous with a single extremum: the cases ±1 and ±2; or with two extrema: the cases ±3, ±4 and ±5. However only one solution is the actual one, verifying the system of equations (8).

Integral form for the system of equations

If we take α instead of ξ as an independent variable, the equations (8.1) and (8.2) become equations with separable variables directly integrable. We may write eq. (8.2) as $d\xi = d\alpha / F(\alpha,A,B,D,Q)$ where $F(\alpha,A,B,D,Q) = S(d\alpha / d\xi)\sqrt{f(\alpha,A,B,D,Q)}$. The integration, between initial value $\alpha(0)$ and final value $\alpha(1)$, can be directly performed only for the case of a structure with monotonous variation of the tilt angle (labelled with 0 in Table I). All the other types of solutions involve at least one extremum of tilt angle (of type $\pm\alpha_M$ or $\pm\alpha_m$), for which $F(\alpha,A,B,D,Q)=0$. In this case the integrands diverge when α approach one extremum value. In Appendices A and B, some substitution that put in evidence the extremum tilt angle allowing to avoid the

divergence of integrands are made. Then the particular mode of writing the integrals for the regions of cell which contain an extremum of tilt angle, is presented. For the types of solutions ±1, respectively ±2, the integration path covers all the cell with substitution and limits given in Appendices A, B, respectively and from Table I. On account that the solutions ±3, ±4 and ±5 involve two extrema of tilt angle, two integrating intervals in the cell thickness have to be considered. In this case, we consider a limit of separation between intervals situated in a position in which α, after passing the first extremum, comes back to the value $\alpha(0)$. The second integration interval has the values $\alpha(0)$ and $\alpha(1)$ at limits and contains the second extremum. In these cases, the substitutions and the limits of integration are used over the adequate intervals, according to Table I and the Appendices A and B.

So, the system that allows the determination of set of structural parameters $\Re=\Re[A,B,D,Q,\alpha(0),\beta(0),\alpha(1),\beta(1)]$, for the extremum free energy structures can be generally written as:

$$\sum_{j=1}^{N}\int_{\alpha(ini_j)}^{\alpha(fin_j)}\frac{B+Q\cdot\cos^2\alpha}{\left(1+b\cdot\sin^2\alpha\right)\cdot\cos^2\alpha}\cdot\frac{d\alpha}{F[\alpha,A,B,D,Q]}=\beta(1)-\beta(0) \tag{9.1}$$

$$\sum_{j=1}^{N}\int_{\alpha(ini_j)}^{\alpha(fin_j)}\frac{d\alpha}{F[\alpha,A,B,D,Q]}=1 \tag{9.2}$$

$$\sigma(0)\cdot\frac{2\pi K_{11}}{QP}\cdot\left(1+a\cdot\sin^2\alpha(0)\right)\cdot F[\alpha(0),A,B,D,Q]=\frac{\partial W_S[\alpha(0),\beta(0),\alpha_0,\beta_0]}{\partial\alpha(0)} \tag{9.3}$$

$$\frac{2\pi K_{11}}{QP}\cdot c\cdot B=\frac{\partial W_S[\alpha(0),\beta(0),\alpha_0,\beta_0]}{\partial\beta(0)} \tag{9.4}$$

$$-\sigma(1)\cdot\frac{2\pi K_{11}}{QP}\cdot\left(1+a\cdot\sin^2\alpha(1)\right)\cdot F[\alpha(1),A,B,D,Q]=\frac{\partial W_S[\alpha(1),\beta(1),\alpha_1,\beta_1]}{\partial\alpha(1)} \tag{9.5}$$

$$-\frac{2\pi K_{11}}{QP}\cdot c\cdot B=\frac{\partial W_S[\alpha(1),\beta(1),\alpha_1,\beta_1]}{\partial\beta(1)} \tag{9.6}$$

where:

- N in sums represents the number of integration intervals;
- $\alpha(ini_j)$ and $\alpha(fin_j)$ represents the integration limits for the j integration interval, where the case;
- $\sigma(0)$ and $\sigma(1)$ are the signs for bulk distortion derivatives at the limits;

and has the values given in Table 1 for each structure type.

Knowing the set of structural parameter $\mathfrak{R}$ -solution of the system (9)- the free energy of structure and the voltage at which it appears can be calculated:

$$\frac{G}{Area}=\frac{2\pi K_{11}}{QP}\left[\frac{A}{2}+\frac{c\cdot Q^2}{2}-c\cdot Q\cdot\sum_{j=1}^{N}\int_{\alpha(ini_j)}^{\alpha(fin_j)}\frac{B+Q\cdot\cos^2\alpha}{1+b\cdot\sin^2\alpha}\cdot\frac{d\alpha}{F[\alpha,A,B,D,Q]}\right]+W_S(0)+W_S(1) \qquad (10)$$

$$U=\int_0^L E_z dz=D_z\cdot\int_0^L\frac{dz}{\varepsilon_{||}\sin^2\alpha+\varepsilon_{\perp}\cos^2\alpha}=$$

$$=U_0\cdot D\cdot\sum_{j=1}^{N}\int_{\alpha(ini_j)}^{\alpha(fin_j)}\frac{1}{1+d\cdot\sin^2\alpha}\cdot\frac{d\alpha}{F[\alpha,A,B,D,Q]} \qquad (11)$$

In Appendices A, B and C the calculating mode of the variation of tilt angle, α, and azimuthal angle, β, with reduced height, ξ, for an extreme free energy structure corresponding to known parameters, is presented.

DISCUSSION

It is noteworthy that eight structural parameters A, B, D, Q, $\alpha(0)$, $\beta(0)$, $\alpha(1)$ and $\beta(1)$, should be estimated each time, while the system (9) contains only six equations. One of the parameters must be considered constant. The role of the constant parameter is played by:

- The field parameter D, which is zero in the case of structures appearing in the absence of the electric field (U=0), according to equation (11);
- The thickness parameter Q, for the case of structures that appear in the presence of the electric field, because the case of a voltage applied to a wedge cell has no practical interest.

Apart from the constant parameter, any of the parameters may be considered as independent, having a given value at a certain moment, so that the system (9) gives the other parameter values vs. the independent one.

By a continuous variation of the independent parameter, a characteristic curve, relating the parameters of each extremum free energy orientational structure, can be obtained. When we build the characteristic curve, any other structural parameter may assume the role the independent parameter, due to the turning back points, possible to appear for the current independent parameter in a certain part of the characteristic curve. In the same time discontinuities are expected to appear for the surface

orientation parameters [$\beta(0)$, $\beta(1)$, $\alpha(0)$ or $\alpha(1)$] when the independent parameter is continuously varied. These discontinuities must be compatible with the symmetry $\vec{n} = -\vec{n}$ of the liquid crystal. The characteristic curve has portions corresponding to the minimum, as well as to the maximum, free energy orientational structures.

In the particular case of (non-chiral) nematics, $P=\infty$ and $Q=0$. Therefore we have to turn back to the dimensional structural parameter, L, in all the equations in which the product QP appears.

An extreme value of the tilt angle is not recommended to be used as a general structural parameter due to the following:

- First, an extreme value is not present for the structures with monotonous variations of tilt angle;
- Second, when a structure with two extreme values of the tilt angle appears, we have not only to choose the parameter between these values, but also to specify their succession.

However, the values of the extreme tilt angles (when they exist), as well as the specification of the structure type, or the position of the extreme tilt angles inside the cell possess all a physical significance. They can be obtained from the set of parameters $\mathfrak{R}$ according to the next procedure. The roots of the function f as defined by equation (8.2) are the first to be determined, giving the possible extremes. Then, we have to choose the actual solution among the five types of solutions allowed by these roots and the superficial tilt angles $\alpha(0)$ and $\alpha(1)$, using system (9). For the actual solution the amounts with physical significance such as free energy of the structure, voltage, or the actual mode of variation for the tilt and azimuthal angles, now become possible to be calculated.

The above procedure must be followed when the characteristic curve is to be calculated. The boundary conditions involved by parameters $\alpha(0)$ and $\alpha(1)$ as well as the values of the possible extreme angles, given by the roots of the function f, are varying when the variation of the independent parameter occurs. Either the spectrum of possible types of solutions or the actual type may change in this process. The computation of the characteristic curve is an extrapolating process, so that the variation of the independent parameter gives approximate values for the other parameters, which must be improved to fulfil system (9). When the actual solution type corresponding to the new exact set of parameters changes, two solution types are near to fulfil the system (9), and special care must be taken during the improvement of the approximate parameter set.

Another question concerns the justification of the presence of all orientational

structures in Table I. The structures labelled with negative figures, having at least one extreme tilt angle with negative values, are the first to be analysed. Angles of negative tilt anchoring $\alpha(S)$ may exist since $\vec{n} = -\vec{n}$, namely $\vec{n}(\alpha,\beta) = \vec{n}(-\alpha,\beta \pm \pi)$. Therefore, if one of the surface anchoring angles has a negative value and its modulus is higher than those of the angle of anchoring at the other surface, a structure of the type -1 may be considered. The type -2 structure involves not only both anchoring angles being negative, but also the tilt angle in the whole bulk to be negative. Of course, this structure type can be transformed in a structure of type +2 (having all tilt angles positive) by redefining the director orientations on the surface and in bulk, following anti parallel directions. The type -2 of orientational structure can have neighbouring structures on the characteristic curve, for which orientation redefining is not suitable or implies too many jumps of surface parameters when going on the characteristic curve. One can give arguments supporting the idea to consider structures with two extremes of the tilt angles. These structures may appear as structures of extreme (not necessarily minima) free energy on a certain portion of the characteristic curve, mainly in the case when the easy axes of surfaces have different tilt angles. These can have neighbouring structures with only one extreme tilt angle (these later not necessarily minimum of free energy). In this manner, the continuity of structural parameters among the structures of minimum free energy is assured.

CONCLUSIONS

In this paper we have reported an analysis and a computing mode of the structures corresponding to the extreme free energy, in the general case of a cholesteric liquid crystal layer, submitted to an electric field, for weak, tilted, different at the two boundary surfaces anchoring. All simple types of structures have been classified, and characterised in a unitary manner by a set of structural parameters. The system of equations, necessary to find the set of structural parameters, and the corresponding director field were written in an integral form ready for use in numerical calculations.

APPENDIX A The solution in the region that contains an extreme tilt angle of α_M type

Let us consider a liquid crystal layer region bounded by the reduced heights $\xi(ini)$ and $\xi(fin)$ which includes an extreme tilt angle of type $\pm\alpha_M$, and only one. Let be $\alpha(ini)$

and $\alpha(fin)$ the tilt angles and $\beta(ini)$ and $\beta(fin)$ the azimuthal angles at the boundary of the layer. Taking into account that for $\alpha=\pm\alpha_M$ we have $\dot{\alpha} = 0$ then:

- to stress the passing of the tilt angle through the extreme value $\pm\alpha_M$,
- to perform the integrals involved in equations (9-11), avoiding, in the same time the divergence that function $F[\alpha,A,B,D,Q]$ introduces when $\alpha\rightarrow\pm\alpha_M$,
- to change the variable with non-monotonous variation, α, by a monotonous one, some substitutions are necessary. These one are:
- the structural parameter A is linked by extreme tilt angle, α_M by:

$$A = c\cdot\frac{\left(B+Q\cdot\cos^2\alpha_M\right)^2}{(1+b\cdot\sin^2\alpha_M)\cos^2\alpha_M}-\frac{D^2}{d}\cdot\frac{S(d)}{1+d\cdot\sin^2\alpha_M} \tag{A.1.1}$$

- the structural variable α is substituted to a variable φ defined by:

$$\sin\alpha = \sin\alpha_M\cdot\sin\varphi \tag{A.1.2}$$

For some constants and functions we use the following notations:

$$\left.\begin{aligned}
&\Psi_M=\sin^2\alpha_M,\quad \Phi_M(\varphi)=\sin^2\alpha_M\cdot\sin^2\varphi,\\
&T1=\frac{S(d)\cdot D^2}{1+d\cdot\Psi_M},\quad T2=c\cdot\frac{B^2}{1-\Psi_M},\quad T3=-c\cdot\frac{b\cdot B^2+[1-\Psi_M]\cdot Q\cdot[(b+1)\cdot Q+2\cdot b\cdot B]}{[1+b\cdot\Psi_M]\cdot[1-\Psi_M]},\\
&F_M[\varphi,\alpha_M(A),B,D,Q]=\sqrt{\frac{T1\cdot[1-\Phi_M(\varphi)]}{1+d\cdot\Phi_M(\varphi)}+\frac{T2+[1-\Phi_M(\varphi)]\cdot T3}{1+b\cdot\Phi_M(\varphi)}},\\
&\Theta(\alpha)=\arcsin(\sin\alpha/\sin\alpha_M).
\end{aligned}\right\} \tag{A.2}$$

We note the limits of integrals, as follows:

- if the region contains an extreme of type α_M, then in the integrals we put as limiting values $\omega(ini)=\Theta(\alpha(ini))$ and $\omega(fin)=\pi-\Theta(\alpha(fin))$,
- if the region contains an extreme of type $-\alpha_M$, then in the integrals we put as limiting values $\omega(ini)=\pi-\Theta(\alpha(ini))$ and $\omega(fin)=2\pi+\Theta(\alpha(fin))$.

Under these conditions the contribution of the region to the different equations can be written as follows:

- at the equation (9.1):

$$\int_{\omega(ini)}^{\omega(fin)}\frac{B+Q\cdot[1-\Phi_M(\varphi)]}{[1+b\cdot\Phi_M(\varphi)]\cdot[1-\Phi_M(\varphi)]}\cdot\frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.3.1}$$

- at the equation (9.2):

$$\int_{\omega(ini)}^{\omega(fin)} \frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.3.2}$$

- at the equations (9.3) and/or (9.5) the region contributes, where it is the case, with the sign, σ, according to the Table I;

- at the equation (10) which give the free energy:

$$\int_{\omega(ini)}^{\omega(fin)} \frac{B+Q\cdot[1-\Phi_M(\varphi)]}{1+b\cdot\Phi_M(\varphi)}\cdot\frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.4}$$

- at the equation (11) which gives the voltage:

$$\int_{\omega(ini)}^{\omega(fin)} \frac{1}{1+d\cdot\Phi_M(\varphi)}\cdot\frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.5}$$

The link between the tilt angle, α, the azimuthal angle, β, and the reduced height, ξ, can be written by means of a parameter Ω:

$$\alpha=\alpha(ini)+\int_{\omega(ini)}^{\Omega}\sqrt{\frac{\Psi_M-\Phi_M(\varphi)}{1-\Phi_M(\varphi)}}\cdot S(\pi/2-\varphi)\cdot S(3\pi/2-\varphi)\cdot d\varphi \tag{A.6.1}$$

$$\beta=\beta(ini)+\int_{\omega(ini)}^{\Omega}\frac{B+Q\cdot[1-\Phi_M(\varphi)]}{[1+b\cdot\Phi_M(\varphi)]\cdot[1-\Phi_M(\varphi)]}\cdot\frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.6.2}$$

$$\xi=\xi(ini)+\int_{\omega(ini)}^{\Omega}\frac{d\varphi}{F_M[\varphi,\alpha_M(A),B,D,Q]} \tag{A.6.3}$$

where Ω takes values from ω(ini) to ω(fin), and the function S, from (A.1.1), (A.2) and (A.6.1), is the sign function defined in (6).

APPENDIX B The solution in the region that contains an extreme tilt angle of α_m type

Let us consider a liquid crystal layer region bounded by the reduced heights ξ(ini) and ξ(fin) which includes an extreme tilt angle of type $\pm\alpha_m$, and only one. Let be α(ini) and α(fin) the tilt angles and β(ini) and β(fin) the azimuthal angles at the boundary of the layer. Taking into account that for $\alpha=\pm\alpha_m$ we have $\dot{\alpha}=0$ then:

- to stress the passing of the tilt angle through the extreme value $\pm\alpha_m$,
- to perform the integrals involved in equations (9-11), avoiding, in the same time

the divergence that function $F[\alpha,A,B,D,Q]$ introduces when $\alpha \to \pm\alpha_m$,

- to change the variable with non-monotonous variation, α, by a monotonous one, some substitutions are necessary. These one are:

- the structural parameter A is linked by extreme tilt angle, α_m by:

$$A = c \cdot \frac{\left(B + Q \cdot \cos^2 \alpha_m\right)^2}{(1 + b \cdot \sin^2 \alpha_m)\cos^2 \alpha_m} - \frac{D^2}{d} \cdot \frac{S(d)}{1 + d \cdot \sin^2 \alpha_m} \tag{B.1.1}$$

- the structural variable α is substituted with variable φ defined by:

$$\cos\alpha = \cos\alpha_m \cdot \cos\varphi \tag{B.1.2}$$

For some constants and functions we will use the following notations:

$$\left.\begin{aligned}
&\Psi_m = \cos^2 \alpha_m, \quad \Phi_m(\varphi) = \cos^2 \alpha_m \cdot \cos^2 \varphi, \\
&T1 = -\frac{S(d) \cdot D^2}{d + 1 - d \cdot \Psi_m}, \quad T2 = -c \cdot \frac{B^2}{\Psi_m}, \quad T3 = c \cdot \frac{b \cdot B^2 + \Psi_m \cdot Q \cdot [(b+1) \cdot Q + 2 \cdot b \cdot B]}{(b + 1 - b \cdot \Psi_m) \cdot \Psi_m}, \\
&F_m[\varphi, \alpha_m(A), B, D, Q] = \sqrt{\frac{1 - \Phi_m(\varphi)}{a + 1 - a \cdot \Phi_m(\varphi)} \cdot \left[\frac{T1}{d + 1 - d \cdot \Phi_m(\varphi)} + \frac{T2 + T3 \cdot \Phi_m(\varphi)}{\left[b + 1 - b \cdot \Phi_m(\varphi)\right] \cdot \Phi_m(\varphi)}\right]}, \\
&\theta(\alpha) = \arccos\left(\cos\alpha / \cos\alpha_m\right).
\end{aligned}\right\} \tag{B.2}$$

We note the limits of integrals, as follows:

- if the region contains an extreme of type α_m, then in the integrals we put as limiting values $\omega(ini)=-\theta(ini)$ and $\omega(fin)=\theta(fin)$,

- if the region contains an extreme of type $-\alpha_m$, then in the integrals we put as limiting values $\omega(ini)=\pi-\theta(ini)$ and $\omega(fin)=2\pi+\theta(fin)$.

Under these conditions the contribution of this region to the different equations can be written as follows:

- at the equation (9.1):

$$\int_{\omega(ini)}^{\omega(fin)} \frac{B + Q \cdot \Phi_m(\varphi)}{\left[b + 1 - b \cdot \Phi_m(\varphi)\right] \cdot \Phi_m(\varphi)} \cdot \frac{d\varphi}{F_m[\varphi, \alpha_m(A), B, D, Q]} \tag{B.3.1}$$

- at the equation(9.2):

$$\int_{\omega(ini)}^{\omega(fin)} \frac{d\varphi}{F_m[\varphi, \alpha_m(A), B, D, Q]} \tag{B.3.2}$$

- at the equations (9.3) and/or (9.5) the region contributes, where it is the case, with the sign, σ, according to the Table I;

- at the equation (10) which give the free energy:

$$\int_{\omega(ini)}^{\omega(fin)} \frac{B+Q\cdot\Phi_m(\varphi)}{b+1-b\cdot\Phi_m(\varphi)}\cdot\frac{d\varphi}{F_m[\varphi,\alpha_m(A),B,D,Q]} \tag{B.4}$$

- at the equation (11) which gives the voltage:

$$\int_{\omega(ini)}^{\omega(fin)} \frac{1}{d+1-d\cdot\Phi_m(\varphi)}\cdot\frac{d\varphi}{F_m[\varphi,\alpha_m(A),B,D,Q]} \tag{B.5}$$

The link between the tilt angle, α, the azimuthal angle, β, and reduced height, ξ, can be written by means of a parameter Ω:

$$\alpha=\alpha(ini)+\int_{\omega(ini)}^{\Omega}\sqrt{\frac{\Psi_m-\Phi_m(\varphi)}{1-\Phi_m(\varphi)}}\cdot S(\varphi)\cdot S(\pi-\varphi)\cdot d\varphi \tag{B.6.1}$$

$$\beta=\beta(ini)+\int_{\omega(ini)}^{\Omega}\frac{B+Q\cdot\Phi_m(\varphi)}{[b+1-b\cdot\Phi_m(\varphi)]\cdot\Phi_m(\varphi)}\cdot\frac{d\varphi}{F_m[\varphi,\alpha_m(A),B,D,Q]} \tag{B.6.2}$$

$$\xi=\xi(ini)+\int_{\omega(ini)}^{\Omega}\frac{d\varphi}{F_m[\varphi,\alpha_m(A),B,D,Q]} \tag{B.6.3}$$

where Ω takes values from $\omega(ini)$ to $\omega(fin)$, and the function S, from (B.1.1), (B.2) and (B.6.1), is the sign function defined in (6).

APPENDIX C The solution for structures with monotonous variation

In the case of structures with tilt angle monotonous variation between the limits on the surfaces, $\alpha(0)$ and $\alpha(1)$, all the equations containing integrals are easily solved. The equations (9-11) are used with the next observations:

- the integration parameter is α,
- the function $F(\alpha,A,B,D,Q)=S[\alpha(1)-\alpha(0)]\sqrt{f(\alpha,A,B,D,Q)}$ where $f(\alpha,A,B,D,Q)$ is defined in (8.2),
- there is only one domain in the whole cell (N=1).

The link between the tilt angle α, the azimuthal angle β and the reduced height ξ can be expressed by the means of a parameter Ω:

$$\alpha=\Omega \tag{C.6.1}$$

$$\beta = \beta(0) + \int_{\alpha(0)}^{\Omega} \frac{B + Q \cdot \cos^2 \alpha}{(1 + b \cdot \sin^2 \alpha) \cdot \cos^2 \alpha} \cdot \frac{d\alpha}{F[\alpha, A, B, D, Q]} \qquad (C.6.2)$$

$$\xi = \int_{\alpha(0)}^{\Omega} \frac{d\alpha}{F[\alpha, A, B, D, Q]} \qquad (C.6.3)$$

where Ω take values in the interval from $\alpha(0)$ to $\alpha(1)$ and the function S, from (C.6.2) and (C.6.3), is the sign function defined in (6).

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