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Stability of some structures in a cholesteric liquid crystal layer for tilted anchoring

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An analysis of the permitted structures for a cholesteric liquid crystal based on the continuum theory as a function of the anchoring conditions and the thickness of the liquid crystal layer is presented. A new type of bistability is found. The stability domains of various structure types are given.

1. Introduction

The development of liquid crystal displays is based on the study of structures appearing in liquid crystal cells, which leads to the discovery of new electro-optic effects. Until now much interest has been accorded to the appearance of a bistability between two structures, stable in the presence of the electric field or in its absence. In pure nematics, Porte and Jadot [1] and Scheffer [2] first described bistable configurations. Boyd *et al.* [3, 4] discovered bistabilities among topologically distinct planar horizontal, planar vertical and 180° twisted structures. In antisymmetrical anchoring cells, Cheng [5] demonstrated the existence of a configurational bistability between two asymmetric orientation structures, stable above a threshold voltage. Berreman and Heffner [6–8] discovered theoretically and showed experimentally the existence of a bistability between two topologically equivalent structures in cells with cholesteric liquid crystals and oblique molecular anchoring at the boundary surfaces. Switching between the two structures, stable in the absence of the electric field, is done by applying and/or interrupting it. In the switching process the appearance or the motion of some disclinations is not necessary. In large pitch cholesterics, for about 270° twist cells, the existence of a holding voltage bistability has also been reported [9–12].

These papers are concerned with the stability of various structures only for a few intervals of cell thickness and of the director twist angle. The aim of the present paper is to discuss the stability of different structure types for large intervals of cell thickness and at any twist angle.

2. Theory

2.1. *Basic equations*

Let a cholesteric liquid crystal layer, having a pitch P, be confined between two plane-parallel surfaces at $z=0$ and $z=L$. The director orientation at a point inside the liquid crystal layer is denoted by $\mathbf{n}$, determined by the tilt angle α and the twist angle β, so that

$$\mathbf{n}(\alpha, \beta) = (\cos\alpha \cos\beta, \cos\alpha \sin\beta, \sin\alpha). \quad (1)$$

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The distortion free energy per unit area of cell is given by

$$W_d = \frac{1}{2}\int_0^L [K_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n} + 2\pi/P)^2 + K_{33}(\mathbf{n}\times\operatorname{curl}\mathbf{n})^2]\,dz, \tag{2}$$

where K_{11}, K_{22} and K_{33} are the elastic constants. Considering that the director orientation depends only on z, equation (2) can be rewritten as

$$W_d = \tfrac{1}{2}K_{11}(W + cQ^2)/L, \tag{3}$$

where

$$W = \int_0^1 w_s\,d\tau$$

$$w_s = (1 + a\sin^2\alpha)\alpha'^2 + c\beta'[\beta'(1 + b\sin^2\alpha) - 2Q]\cos^2\alpha,$$

$$a = (K_{11} - K_{33})/K_{11}, \quad b = (K_{33} - K_{22})/K_{22}, \quad c = K_{22}/K_{11},$$

$$\tau = z/L, \quad \alpha' = \delta\alpha/\delta\tau, \quad \beta' = \delta\beta/\delta\tau, \quad Q = 2\pi L/P.$$

W will be used as a dimensionless measure of the distortion free energy.

Variational calculus leads to two differential coupled equations which describe the director orientation inside the liquid crystal layer. After a first integration these can be written as:

$$\alpha'^2(1 + a\sin^2\alpha) = f(A, B, Q, \alpha), \tag{4a}$$

$$\beta' = \frac{B + Q\cos^2\alpha}{(1 + b\sin^2\alpha)\cos^2\alpha} \tag{4b}$$

where

$$f(A, B, Q, \alpha) = A - c\frac{(B + Q\cos^2\alpha)^2}{(1 + b\sin^2\alpha)\cos^2\alpha} \tag{5}$$

and A and B are integration constants, which together with Q play the role of constants for a structure with extreme energy. Using equations (4), it is possible to write the free energy corresponding to the structure characterized by the parameters set A, B and Q as

$$W = A - 2cQ\int_0^1 \frac{B + Q\cos^2\alpha}{1 + b\sin^2\alpha}\,d\tau. \tag{6}$$

2.2. *Structure types*

Let the easy orientation of the director at the $z = 0$ boundary be specified by the tilt angle $\alpha(0) = \alpha_0 > 0$ and the azimuthal angle $\beta(0) = 0$. We consider that the easy orientation of the director at the $z = L$ surface can be specified by a tilt angle $0 < \alpha_1 \leqslant \alpha_0$ and an azimuthal mounting angle (AMA) $-\pi < \beta_1 < \pi$. A cholesteric liquid crystal embedded between these two surfaces may take various orientational structures so that the easy direction at the $z = 0$ surface is related to the easy direction at the $z = L$ surface by a continuous variation of the director orientation $\mathbf{n}$. In order to characterize the various structures, we suppose that the director is specified at $z = 0$ by the same parameters $\alpha(0) = \alpha_0$ and $\beta(0) = 0$, for any possible structure. The director at the $z = L$ surface is characterized by the tilt angle α_L and the total twist angle (TTA) β_L, which are related to α_1 and β_1 in a manner depending on orientational structure type, taking into account that $\mathbf{n} = -\mathbf{n}$.

The analysis of the modes in which boundary orientations can be continuously connected shows the possibility of the appearance of three structure types:

(i) *The T-type tilted structure.* This structure is characterized by $0<\alpha(z)<\pi/2$ for any z. At the $z=L$ surface, the director orientation is specified by the tilt angle $\alpha_L=\alpha_1>0$ and a TTA

$$\beta_L=\beta_1+2k\pi \quad \text{with} \quad k=0,\pm 1,\pm 2,\ldots.$$

(ii) *The H-type horizontal structure.* There is a surface $0<z_H<L$ for which $\alpha(z_H)=0$, in this case. The director orientation at $z=L$ is specified by the tilt angle $\alpha_L=-\alpha_1<0$ and a TTA

$$\beta_L=\beta_1+(2k+1)\pi \quad \text{with} \quad k=0,\pm 1,\pm 2,\ldots.$$

(iii) *The V-type vertical structure.* There is a surface $0<z_V<L$ for which $\alpha(z_V)=\pi/2$, in this case. Due to this vertical orientation we cannot speak about a total twist angle for this structure type, since at $z=z_V$ a jump of any value in the $\beta(z)$ function can be introduced. The director at $z=L$ can be specified by $\alpha_L=\alpha_1$ or better by $\alpha_L=\pi-\alpha_1$ to note that the tilt passes through a value of $\pi/2$.

2.3. *Structures of extreme free energy*

To find an extreme free energy solution, that is a solution for equations (4), means to find the structure parameter set A, B and Q corresponding to this solution. The analysis of equations (4) can provide useful information not only about the possibility that a proposed set of A, B and Q parameters corresponds to an extreme energy solution, but also about the mode in which α and β can vary to yield that solution.

A necessary condition for a proposed parameter set to correspond to a possible solution is the right hand member of equation (4 *a*), namely the function f given in equation (5), to be positive for the whole interval in which α varies, in order to relate continuously the values α_0 and α_L at the boundary surfaces. The α values for which $f(\alpha)$ vanishes, situated out of the interval (α_L, α_0), can really represent the maximum, α_M, or the minimum, α_m, values of the tilt angle of the structure corresponding to the A, B, Q parameters, since they lead to $\alpha'=0$.

It must be observed that two or four solution types, depending on the number of roots of $f(\alpha)$ function, seem to correspond to a given parameter set:

(i) one of the solutions corresponds to a monotonous variation of the tilt angle in the interval $[\alpha_L, \alpha_0]$,
(ii) another solution corresponds to a maximum tilt angle α_M situated in the interval $[\alpha_0, \pi/2]$,
(iii) another solution has a minimum tilt angle α_m, situated in the interval $(0, \alpha_1]$ for $\alpha_L>0$ or in the interval $(-\pi/2, -\alpha_0]$ for $\alpha_L<0$,
(iv) the last solution type has both a maximum tilt angle and a minimum one.

However only one of these solution types is an actual solution which gives a continuous connection of the director orientation at the two surfaces, for a given A, B, Q parameter set. To obtain the solution for a V-type structure we must put $B=0$ in equation (4 *a*). In this case, the $f(\alpha)$ function does not diverge when the tilt angle approaches $\pi/2$.

We observe that if the parameter set A, B, Q represents an extreme energy solution for a structure characterized by a TTA β_L, then the set A, $-B$, $-Q$ is a solution for the structure with a TTA $-\beta_L$.

The mode of solving equations (4) for each of the solution types is given in Appendices. Equations (3) and (4) in the corresponding Appendix supply two conditions for the three parameters A, B and Q. They permit us to obtain two of the parameters when the third is fixed. Equations (5) in the Appendices give the energy value for these A, B, Q parameters.

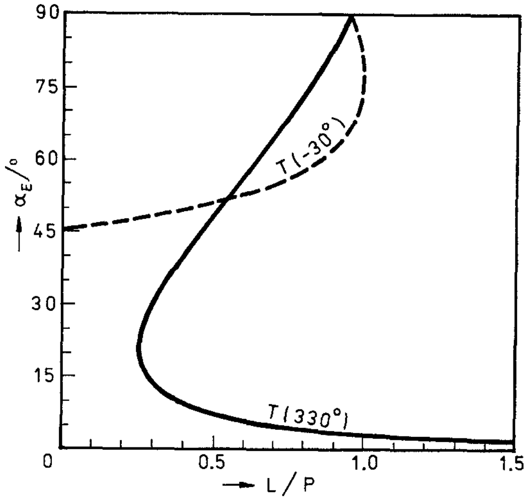
3. Results and discussion

Here we present the results of numerical calculations for the cases in which the superficial liquid crystal orientation at both surfaces is characterized by the same tilt angle $\alpha_0 = \alpha_1$. We consider a cholesteric liquid crystal having the elastic constants of the nematic liquid crystal RO-TN 615 (La Roche). $K_{11} = 10 \times 10^{-7}$ N, $K_{22} = 5{\cdot}2 \times 10^{-7}$ N, $K_{33} = 13{\cdot}9 \times 10^{-7}$ N. For $\alpha_0 = \alpha_1$ the T-type structures having extreme distortion energy can be specified by the extreme tilt angle α_E (maximum, α_M or minimum, α_m). In figure 1, for two AMA $\beta_1 = -30°$ respectively $\beta_1 = -135°$, we present α_E versus the reduced thickness L/P for the first two T-type structures, both being solutions of equations (4) compatible with the boundary conditions $\alpha_0 = \alpha_1 = 45°$ and the same AMA. This figure suggests that, for negative AMA when α_E approaches 90°, we can speak about a continuity of characteristic parameters for the two T-type solution of equations (4) with TTA differing by 360°. This continuity can be better observed for other structural parameters (like A, B, or W). In figure 2 the structure parameter A versus L/P is represented for the T-type structures from figure 1 as well as for the V-type structure which is also a solution of equations (4), compatible with the boundary conditions.

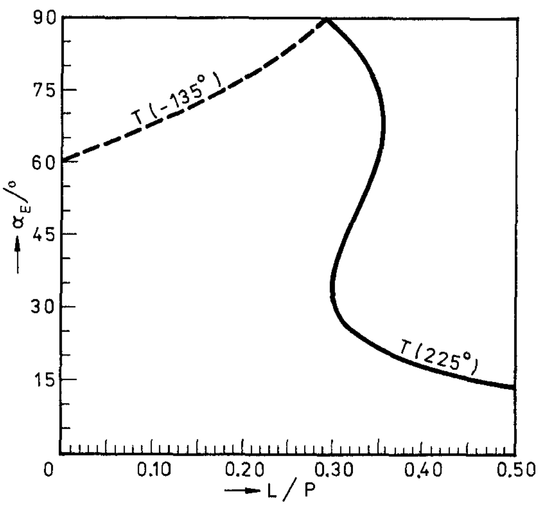
The thickness for which a T-type structure becomes like a V-type one (i.e. for which α_E is about 90°) can sometimes have the meaning of the limiting thickness of existence for that structure (see $L/P = 0{\cdot}3$ in figure 1 (*b*)). The turning points on the characteristic curves act as limiting thicknesses under or above which T-type structures with certain characteristic cease to exist.

In figure 3 the distortion energy versus L/P for the same structures as in figure 1 is represented. By comparing it with figure 2 we can see that to the positive slope portions in A versus L/P curves correspond a smaller distortion energy than to the negative slope portions of the same curves. The structures having representative points on the portions with positive slope, correspond to minimum distortion energy and are physically realizable ones. When two stable structures, compatible with the same AMA, appear at a certain thickness these structures have very different α_E and accordingly we can speak about an up (T_u) and a down (T_d) structure i.e. either these structures have the same TTA or they have TTA differing by 360° structures.

As the structures having representative points on the negative slope portions of the A versus L/P curves correspond to the greatest energy for the same thickness, they may be considered as barrier structures between the up and down structures. The barrier structure has the same TTA as at least one of the two stable structures. By applying an external adequate field, we may induce the transition from one of the stable structures to the other only if the initial one has the same TTA as the barrier structure. In this case, if the applied field tends to modify the tilt angle of the stable structure towards values which correspond to the barrier structure, then there is a maximum field above which the structure with some characteristic of the stable structure (for example β_L or the up or down character) ceases to exist. If for a stable T-type structure, having a given TTA there is a corresponding barrier having another TTA, then the transition towards the



(*a*)



(*b*)

Figure 1. Dependence of the extreme tilt angle α_E on the reduced thickness for two T-structures corresponding to the same AMA: (*a*) $\beta_1 = -30°$, $\alpha_0 = 45°$, $\alpha_1 = 45°$; solid line $\beta_L = 330°$; dashed line $\beta_L = -30°$, (*b*) $\beta_1 = -135°$, $\alpha_0 = 45°$, $\alpha_1 = 45°$; solid line $\beta_L = 225°$; dashed line $\beta_L = -135°$.

other T-type structure is impossible under the field. However this can appear at the interruption of the field, if the field is strong enough so that, at its interruption, the hydrodynamic effects of reorientation are able to accomplish the transition [6].

Generally we can speak about the appearance of two bistability types between structures of T-type. Berreman and Heffner [7] showed the existence of a first type of bistability, namely between two T-type structures having TTA differing by 360°. This bistability type is represented in figures 1–3 by curves corresponding to the structures having $\beta_L = -30°$ and $\beta_L = 330°$. A new bistability type, not yet mentioned in the

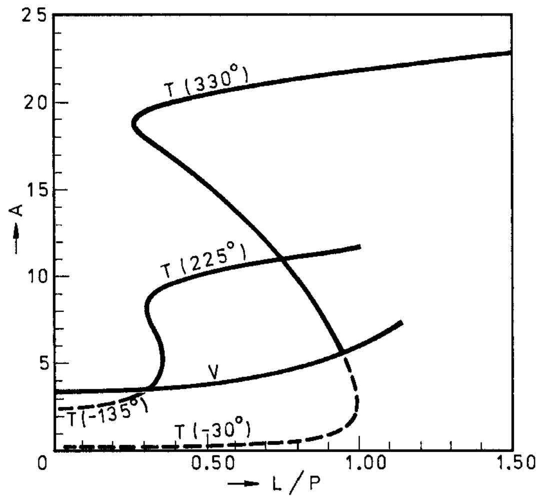


Figure 2. Characteristic parameter A versus the reduced thickness for the first two T-type structures associated with the same AMA, $\beta_1 = -30°$ respectively $\beta_1 = -135°$, and for the V-type solution of equation (4). $\alpha_0 = 45°$, $\alpha_1 = 45°$.

literature, involves stable structures with the same TTA (for example structures corresponding to $\beta_L = 225°$). Because the up, down and barrier structures have the same TTA, the transitions between the stable structures can be made under an applied field in both senses (for example under an electric field for a material having dielectric anisotropy that changes sign when the frequency is changed).

In figure 3 we can see the thickness intervals for which various types of structures are the most stable. The intersection between the curves corresponding to a T-type and a H-type structure gives the reduced thickness at which a Grandjean–Cano disclination is placed inside a wedge cell. Intersection between curves corresponding to two T-type structures, having different or equal TTA, can give a limiting thickness for the most stable structure between them. This case takes place only if the H-type structures at this thickness have a higher distortion energy than that corresponding to the T-structures or if they have been eliminated in a certain manner [6].

In figure 4 we have represented as phase diagrams the cell construction parameters (thickness, AMA and surface tilt anchoring angles) in which various structure types are the most stable. Inside each domain the structure type together with the corresponding TTA are indicated.

We have marked by dashing the domains in which the new type of bistability between up and down structures with the same TTA appear. The limits of bistability domains toward higher or lesser thicknesses are those values for which the up, and the down structures respectively cease to exist. The domains are limited toward higher AMA by construction conditions under which any of the most stable T-type structures begin to have the character as a V-type structure. We have not included in these figures the domains in which the bistability between structures having TTA differing by 360° can appear.

For small superficial tilt angles the bistability between structures with the same TTA is absent, only the bistability between T-type structures with different twist angles can appear especially if we are able to eliminate the H-type structure.

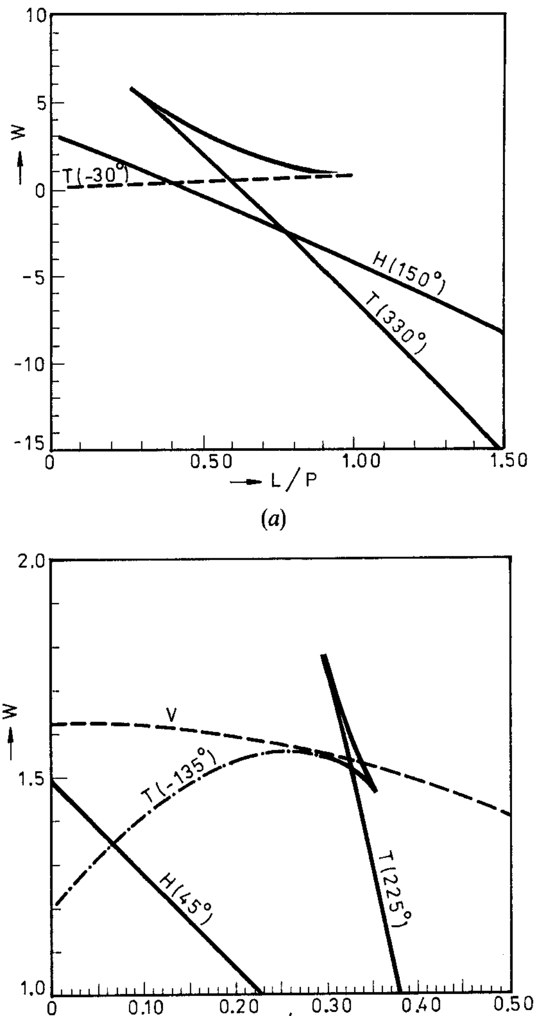
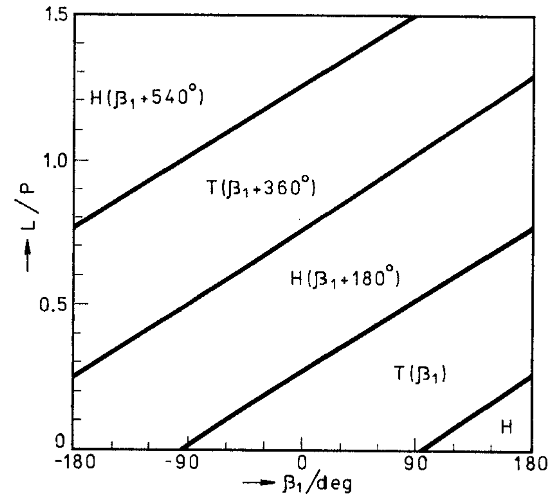


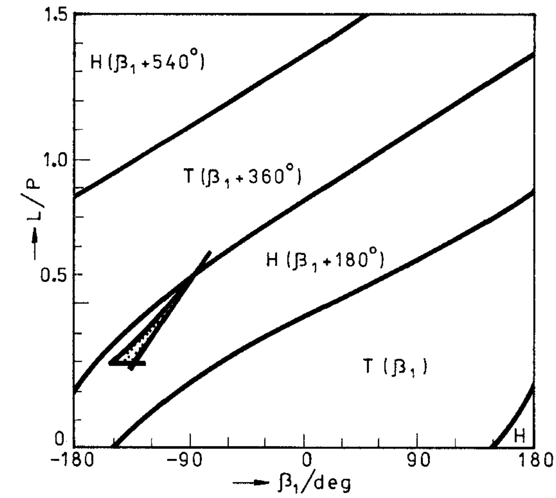
Figure 3. The distortion energy versus the reduced thickness for structures compatible with boundary conditions $\alpha_0 = \alpha_1 = 45°$ and the same AMA: (*a*) $\beta_1 = -30°$; (*b*) $\beta_1 = -135°$.

For superficial tilt angles $\alpha_0 = \alpha_1 = 45°$ bistability between T-type structures with the same TTA becomes possible but its existence domain is embedded in the domain in which the H-type structures are the most stable. Near $\beta_1 = \pm 180°$ we notice the non-linear dependence of the thickness at which the Grandjean–Cano disclinations are placed as a function of AMA.

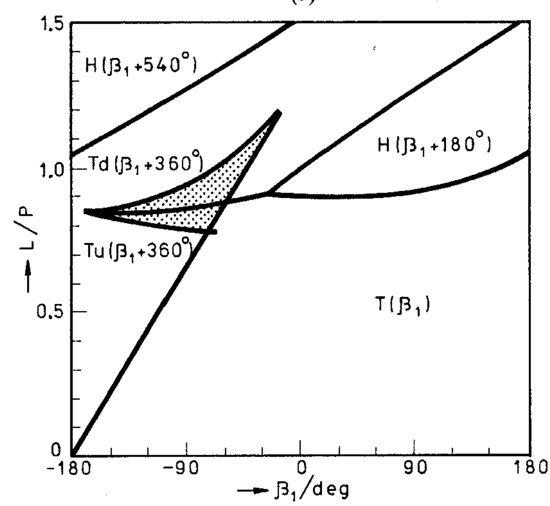
At higher superficial tilt angles the H-type structures disappear for thin cells irrespective of the value of AMA. A V-type-like limit which separates the existence domains for T-type structures with β_L differing by 360° appears in such cells. The T-type structures appearing under these circumstances are the most stable, their distortion energy being even lower than that for V-type structures, in a similar manner as described in figure 3 (*b*). Consequently we cannot assign a domain for V-type structures in our phase diagrams.


H(β1+540°)
T(β1+360°)
H(β1+180°)
T(β1)
H
L/P
β1/deg

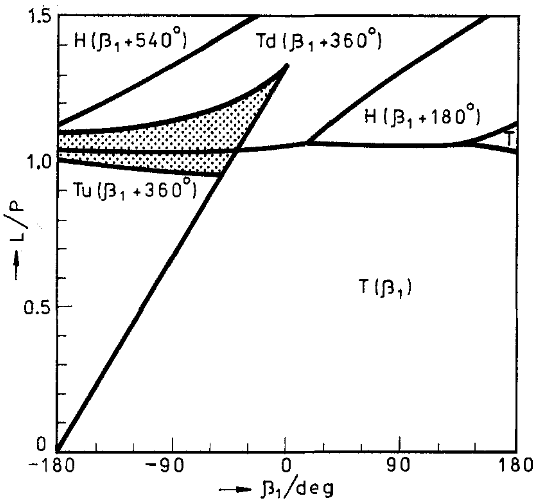
(*a*)


H(β1+540°)
T(β1+360°)
H(β1+180°)
T(β1)
H
L/P
β1/deg

(*b*)


H(β1+540°)
Td(β1+360°)
Tu(β1+360°)
H(β1+180°)
T(β1)
L/P
β1/deg

(*c*)



(*d*)

Figure 4. Domains of cell construction parameters for the most stable structures in cells having the same tilt angles: (*a*) $\alpha_0=\alpha_1=15°$; (*b*) $\alpha_0=\alpha_1=45°$; (*c*) $\alpha_0=\alpha_1=75°$; (*d*) $\alpha_0=\alpha_1=85°$. H in the lower right hand corner represents an H-type structure with $\beta_L=\beta_1-180°$ and T the right of (*d*) a down T-type structure with $\beta_L=\beta_1$. In the dashed domains a bistability between up and down T-structures having the same value $\beta_L=\beta_1+360°$ can appear. The line inside the dashed domain represents the line of equal energy of the T_u and T_d structures.

4. Conclusions

Here we have presented the mode for describing the orientational structures characterized by extreme values of free energy for a cholesteric liquid crystal confined by plane-parallel surfaces which impose different tilted anchoring of the director. The type of structures appearing, as well as the possible modes in which the director orientation can connect, in a continuous manner, the easy directions imposed by the two boundary surfaces are analysed. The appearance of a new type of bistability between two T-type structures having the same total twist angle, but different extreme tilt angles is demonstrated. This type of bistability differs from that described by Berreman and Heffner [6, 7]. We give the intervals of cell thickness in which the different structure types are the most stable and also the intervals of cell thickness in which the new bistability forms appear, when the construction parameter β_1 varies between $-180°$ and $180°$.

Appendix A

Solutions with maximum tilt angle α_M

Taking into account that $\alpha'(\alpha_M)=0$, we make the following substitutions:

$$A=c\frac{(B+Q\cos^2\alpha_M)^2}{(1+b\sin^2\alpha_M)\cos^2\alpha_M},$$

$$\sin\alpha=\sin\alpha_M\sin\phi. \qquad (A\,1)$$

Using the notation

$$Y=\sin^2\alpha_M,\quad X=\sin^2\alpha_M\sin^2\phi,$$

$$\theta_0=\arcsin(\sin\alpha_0/\sin\alpha_M),\quad \theta_1=\arcsin(\sin\alpha_1/\sin\alpha_M),$$

$$F_M=\left[c\frac{B_2[b(Y+X)-b+1]-[2bBQ+(b+1)](1-Y)(1-X)}{(1+aY)(1+bY)(1-Y)(1+bX)}\right]^{-1/2} \qquad \text{(A 2)}$$

we integrate equations (4) and obtain for the extreme free energy structure

$$\int_{\theta_0}^{\pi-\theta_1} F_M d\phi=1, \qquad \text{(A 3)}$$

$$\int_{\theta_0}^{\pi-\theta_1} \frac{B+Q-QX}{(1+bX)(1-X)}d\phi=\beta_L. \qquad \text{(A 4)}$$

The free energy can then be expressed as

$$W=A-2cQ\int_{\theta_0}^{\pi-\theta_1}\frac{B+Q-QX}{1+bX}F_M d\phi. \qquad \text{(A 5)}$$

Appendix B

Solutions with minimum tilt angle α_m

Taking into account that $\alpha'(\alpha_m)=0$, we make the following substitutions

$$A=c\frac{(B+Q\cos^2\alpha_m)^2}{(1+b\sin^2\alpha_m)\cos^2\alpha_m},$$

$$\cos\alpha=\cos\alpha_m\cos\phi. \qquad \text{(B 1)}$$

Using the notation

$$a'=a+1,\quad b'=b+1,\quad d'=d+1,\quad y=\cos^2\alpha_m,\quad x=\cos^2\alpha_m\cos^2\phi,$$

$$\theta_0=\arccos(\cos\alpha_0/\cos\alpha_m),\quad \theta_1=\arccos(\cos\theta_1/\cos\theta_m),$$

$$F_m=\left[c(1-x)\frac{B^2[b(y+x)-b']+[2bBQ+b'Q^2]xy}{(a'-ax)(b'-by)(b'-bx)xy}\right]^{-1/2}, \qquad \text{(B 2)}$$

we integrate equations (4) and obtain for the extreme energy structure

$$\int_{-\theta_0}^{\theta_1} F_m d\phi=1, \qquad \text{(B 3)}$$

$$\int_{-\theta_0}^{\theta_1}\frac{B+Qx}{(b'-bx)x}F_m d\phi=\beta_L. \qquad \text{(B 4)}$$

The free energy can then be expressed as

$$W=A-2cQ\int_{-\theta_0}^{\theta_1}\frac{B+Qx}{b'-bx}F_m d\phi. \qquad \text{(B5)}$$

Appendix C

Solutions with monotonous dependence of the tilt angle

In this case equations (4) can be integrated directly using the notation

$$F_{\text{Mon}}=\left[\frac{1+a\sin^2\alpha}{f(A,B,Q,\alpha)}\right]^{1/2}, \tag{C 2}$$

where $f(A,B,Q,\alpha)$ was defined in equation (5), we obtain by integration of equations (4)

$$\int_{\alpha_L}^{\alpha_0} F_{\text{Mon}}\,d\alpha=1, \tag{C 3}$$

$$\int_{\alpha_L}^{\alpha_0}\frac{B+Q\cos^2\alpha}{(1+b\sin^2\alpha)\cos^2\alpha}F_{\text{Mon}}\,d\alpha=\beta_L \tag{C 4}$$

and the free energy expression becomes

$$W=A-2cQ\int_{\alpha_L}^{\alpha_0}\frac{B+Q\cos^2\alpha}{1+b\sin^2\alpha}F_{\text{Mon}}\,d\alpha. \tag{C 5}$$

Appendix D

Solutions with two extrema of the tilt angle

The integration of equations (4) and (6) can be performed by dividing the cell thickness into two intervals, one of them containing the maximum tilt angle α_M orientation (and having α_0 and α_1 as limiting angles), and the other one containing the minimum tilt angle α_m orientation (and having α_1 as limiting angles at the two boundaries). The substitutions and notation in these intervals being those used in Appendices A and B, we obtain by integration of equations (4)

$$\int_{\theta_0}^{\pi-\theta_1}F_M\,d\phi+\int_{-\theta_1}^{\theta_1}F_m\,d\phi=1, \tag{D 3}$$

$$\int_{\theta_0}^{\pi-\theta_1}\frac{B+Q-QX}{(1+bX)(1-X)}F_M\,d\phi+\int_{-\theta_1}^{\theta_1}\frac{B+Qx}{(b'-bx)x}F_m\,d\phi=\beta_L \tag{D 4}$$

and the free energy equation (6) becomes

$$W=A-2cQ\int_{\theta_0}^{\pi-\theta_1}\frac{B+Q-QX}{1+bX}F_M\,d\phi-2cQ\int_{-\theta_1}^{\theta_1}\frac{B+Qx}{b'-bx}F_m\,d\phi. \tag{D 5}$$

Appendix E

Solutions for V-type structures

To find a V-type solution of equations (4) it is necessary that the function $f(A,B,Q,\alpha)$ given by equation (5) ceases to diverge when α approaches $\pi/2$. This is possible when $B=0$. In this instance, equations (4 *a*) and (4 *b*) become uncoupled. At the same time, we consider that the tilt angle at the two surfaces is α_0 and $\pi-\alpha_1$. Using the notation

$$F_V=\left[\frac{1}{1+a\sin^2\alpha}\left(A+c\frac{Q^2\cos^2\alpha}{1+b\sin^2\alpha}\right)\right]^{-1/2} \tag{E 2}$$

we obtain by integration of equation (4 *a*)

$$\int_{\alpha_0}^{\pi-\alpha_1} F_V \, d\alpha = 1. \tag{E 3}$$

The integration of equation (4 *b*) gives

$$\int_{\alpha_0}^{\pi-\alpha_1} \frac{Q}{1+b\sin^2\alpha} F_V \, d\alpha = \beta_t, \tag{E 4}$$

which does not signify the total twist angle of the structure as for the other types of structures. In this case it gives information about the continuous total variation of the azimuthal angle β, knowing that a discontinuity of any value can be added to β, when $\alpha = \pi/2$. Equation (6) becomes for the V-type structure

$$W = A - 2cQ^2 \int_{\alpha_0}^{\pi-\alpha_1} \frac{1}{1+b\sin^2\alpha} \, d\alpha. \tag{E 5}$$

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