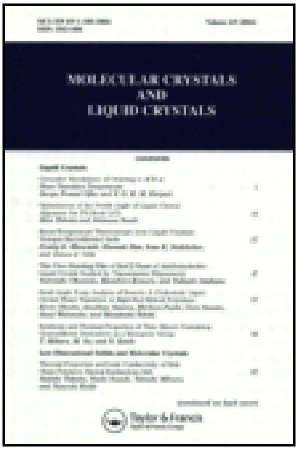

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Periodic Distorted Nematic Director Structures in the Intermediate FrÉedericksz Transition Geometries

J. L. Figueirinhas [a] , L. N. Gonçalves [b] & J. P. Casquilho [c]

[a] Dept. de Fisics, IST, CFMC-UL, Av. Prof. Gama Pinto 2, Lisboa, Codex, Portugal, Lisboa Codex, 1649-003, Portugal

[b] Dept. Fisica FCT/UNL, Caparica, CFMC-UL, Av. Prof. Gama Pinto 2, Lisboa, Codex Portugal, 1649-003, Portugal

[c] Dept. Fisica, FCT/UNL, Quinta da Torre, Caparica, Portugal and CENIMAT, Caparica, 2829-516, Portugal

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PERIODIC DISTORTED NEMATIC DIRECTOR STRUCTURES IN THE INTERMEDIATE FRÉEDERICKSZ TRANSITION GEOMETRIES

J. L. Figueirinhas
CFMC-UL, Av. Prof. Gama Pinto 2,
1649-003 Lisboa, Codex, Portugal and Dept. de Fisics, IST,
Av. Rovisco Pais, 1049-001 Lisboa Codex, Portugal

L. N. Gonçalves
CFMC-UL, Av. Prof. Gama Pinto 2,
1649-003 Lisboa, Codex Portugal and Dept. Fisica, FCT/UNL,
Quinta da Torre, 2829-516 Caparica, Portugal

J. P. Casquilho
Dept. Fisica, FCT/UNL, Quinta da Torre,
2829-516 Caparica, Portugal and CENIMAT, Quinta da Torre,
2829-516 Caparica, Portugal

The occurrence of periodically distorted director structures in planar and pre-tilted nematic slabs above the magnetically driven Fréedericksz transition is investigated in the intermediate geometries between the pure splay, twist and bend Fréedericksz transition geometries. Considering rigid boundary conditions the domain of existence of the periodic structures is determined as a function of the Frank elastic constants ratios K_2/K_1, K_1/K_3 and the magnetic field orientation. It is found that the periodic distorted state can be reached either directly from the undistorted state on increasing the magnetic field or indirectly through the homogeneously distorted state when pre-tilt is present. It is also found in pre-tilted slabs that the transition from the undistorted state to the homogeneously distorted state can be either continuous or discontinuous, and the corresponding lines of tricritical points are determined.

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Address correspondence to J. L. Figueirinhas, CFMC-UL, Av. Prof Gama Pinto 2, 1649-003, Lisboa, Codex, Portugal.

1. INTRODUCTION

The occurrence of periodically distorted nematic director structures above the magnetically driven Fréedericksz transition has been studied both experimentally and theoretically by several authors since the mid seventies. Initiated with the work on the bend geometry by Cladis and Torza [1] and widened with the more recent work on the splay geometry by Lonberg and Meyer [2] the studies on this subject continue to uncover new and relevant features [3–10]. Recently we studied the intermediate geometries between the pure splay and twist and splay and bend geometries [9,10], allowing to expand earlier studies [4–8] and to bring forward new and in-depth results on the conditions of occurrence of periodic structures in those geometries. In this work we extend the studies to the intermediate geometry between the pure twist and bend Fréedericksz transition geometries (I) and give an overall account of the conditions for occurrence of periodically distorted nematic director structures above the magnetically driven Fréedericksz transition in the three intermediate geometries respectively in between the twist and bend (I), the splay and bend (II) and the splay and twist (III). In this study rigid boundary conditions and the absence of flexoelectricity were assumed.

2. CALCULATION METHOD

The approach followed consists in the study of the stability of the nematic director field defined by the angles θ and ϕ which are composed of a non-periodic main term minimising the free energy plus magnetic contribution in between the substrates, and an in-plane periodic perturbation expressed by its x-y spatial Fourier components allowing for the existence of a periodic structure with wave vector in the x, y plane. The nematic director-magnetic field geometry studied is shown in Figure 1. The director considered is:

$$n_x = \cos(\theta+\gamma)\cos(\phi), \quad n_y = \cos(\theta+\gamma)\sin(\phi), \quad n_z = \sin(\theta+\gamma). \quad (1)$$

with θ and ϕ given by:

$$\theta = \sum_{j=1}^{N_0} \theta_{0j}\sin(j\pi z/l) + \Delta\theta \quad (2a)$$

$$\Delta\theta = \cos(\vec{q}.\vec{\rho}/l)\sum_{k=1}^{N_1}\theta_{1k}\sin(k\pi z/l) + \sin(\vec{q}.\vec{\rho}/l)\sum_{k=1}^{N_1}\theta_{2k}\sin(k\pi z/l) \quad (2b)$$

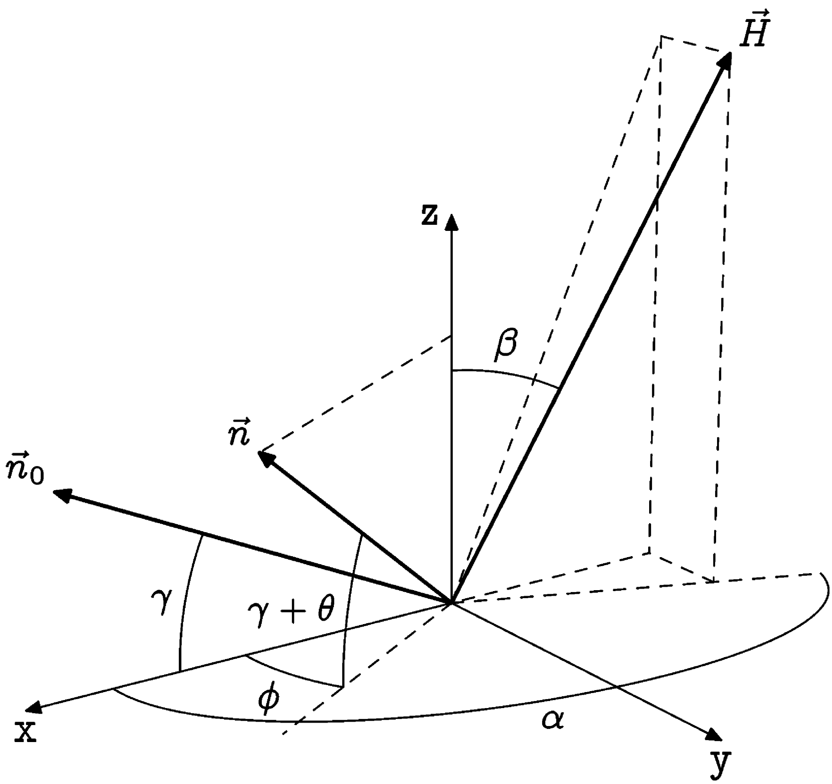

FIGURE 1 Magnetic field and director orientations. The plates are at z = 0 and l.

$$\phi = \sum_{j=1}^{N_0} \phi_{0j} \sin(j\pi z/l) + \Delta\phi \tag{2c}$$

$$\Delta\phi = \cos(\vec{q}.\vec{\rho}/l) \sum_{k=1}^{N_1} \phi_{1k} \sin(k\pi z/l) + \sin(\vec{q}.\vec{\rho}/l) \sum_{k=1}^{N_1} \phi_{2k} \sin(k\pi z/l) \tag{2d}$$

$$\vec{q} = q_x\vec{e}_x + q_y\vec{e}_y, \quad \vec{\rho} = x\vec{e}_x + y\vec{e}_y$$

where γ is the pre-tilt angle, l is slab thickness, $\vec{q}$ is the normalised wave vector of the periodic distortion. The amplitudes $\theta_{0\mathrm{j}}$ and $\phi_{0\mathrm{j}}$ parameterise the non-periodic main terms of θ and ϕ respectively and the reminder constitute the periodic perturbation. The index j runs only over odd integers in order to preserve the symmetry of the homogeneous director distortion with the distortion maximum half way in between the substrates located at z = 0 and z = l. The possibility of considering an adjustable number of

Fourier components in the z dependence of both θ and ϕ describing a homogeneous director distortion allows the attainment of the homogeneously distorted director field that minimises the excess free energy within a specified small error limit, being thus equivalent to the numerical solution of the appropriate Euler-Lagrange equations but with higher numerical stability. The amplitudes θ_{1j}, θ_{2j}, ϕ_{1j} and ϕ_{2j} parameterise the periodic perturbation of the director. As we are only seeking the conditions for the onset of stability of the periodic director structures, only the lowest order Fourier components in **q** must be considered in the director perturbation.

The magnetic field is:

$$\vec{H} = H[\sin(\beta)\cos(\alpha)\vec{e}_x + \sin(\beta)\sin(\alpha)\vec{e}_y + \cos(\beta)\vec{e}_z] \qquad (3)$$

For the intermediate geometries of type I, $\alpha = \beta = \pi/2$, of type II, $\alpha = \pi$, $\beta = \gamma$ and of type III, $\alpha = \pi/2$, $\beta = \psi$, $\gamma = 0$. The Frank free energy plus the magnetic contribution per unit of volume is given by:

$$\begin{aligned} \mathrm{F} = \frac{1}{l\lambda}\int_0^{\lambda} ds \int_0^{l} dz \frac{1}{2}\{&\mathrm{K}_1(\nabla.\vec{n})^2 + \mathrm{K}_2(\vec{n}.\nabla\times\vec{n})^2 \\ &+ \mathrm{K}_3(\vec{n}\times\nabla\times\vec{n})^2 - \chi_a(\vec{n}.\vec{H})^2\} \end{aligned} \qquad (4)$$

with $\vec{s} = s\frac{\vec{q}}{\|\vec{q}\|}$ and $\lambda = \frac{2\pi}{\|\vec{q}\|}l$. After the substitution of **n** by (1) and θ and ϕ by (2), F becomes a function of θ_{0j}, θ_{1k}, θ_{2k}, ϕ_{0j}, ϕ_{1k}, ϕ_{2k}, q_x, q_y that parameterise the director field and the control parameters H, K_1, K_2, K_3, χ_a and γ or ψ. For the calculations we used an nondimensional form of F, given by $F_a = F\, l^2/K_3$ for geometries I and II and $F_a = F\, l^2/K_1$ for the geometry III and worked with the reduced magnetic fields for each specific geometry type:

$$\begin{aligned} &\mathrm{I}- \quad h \equiv H\frac{l}{\pi}\frac{\sqrt{\chi_a/\mathrm{K}_3}}{\sqrt{1-\cos^2(\gamma)(1-\mathrm{K}_2/\mathrm{K}_3)}}, \\ &\mathrm{II}- \quad h \equiv H\frac{l}{\pi}\frac{\sqrt{\chi_a/\mathrm{K}_3}}{\sqrt{1-\cos^2(\gamma)(1-\mathrm{K}_1/\mathrm{K}_3)}} \\ &\mathrm{III}- \quad h \equiv H\frac{l}{\pi}\sqrt{\chi_a/\mathrm{K}_1}\sqrt{1-\sin^2(\psi)(1-\mathrm{K}_1/\mathrm{K}_2)} \end{aligned} \qquad (5)$$

which correspond for h=1 to the stability limit of the undistorted state against the onset of a homogenous distortion as shown in [12].

Our analysis of the intermediate geometry begins with the calculation of the relation between h, K_1/K_3, K_2/K_1 and γ or ψ valid at the stability limit of the undistorted state against the onset of a periodic distortion. In order to obtain the Hessian or stability matrix of F_a with respect to the amplitudes of the periodic perturbation, we consider the expansion of F_a about the desired non perturbed director field to second order in those amplitudes which are θ_{1k}, θ_{2k}, ϕ_{1k}, ϕ_{2k}. In the undistorted state the unperturbed director $\vec{n}$ is uniform and is characterised by $\theta = \phi = 0$ and the stability matrix is:

$$S_{ij} \equiv \left.\frac{\partial^2 F_a}{\partial x_i \partial x_j}\right|_{x_k=0} \qquad x_i = \theta_{1k}, \theta_{2k}, \phi_{1k}, \phi_{2k} \ (\mathrm{k} = 1..\mathrm{N}_1) \tag{6}$$

At the stability limit of the undistorted state the determinant of S_{ij} is zero and this yields an implicit equation that relates the reduced critical magnetic field h with K_1/K_3, K_2/K_1, γ or ψ and the wave vector of the distortion $\vec{q}$. The selected wave vector $\vec{q}$ minimises

$$|S_{ij}| \text{ and from } |S_{ij}|_{\min}(h_1, K_1/K_3, K_2/K_1, \gamma \text{ or } \psi) = 0 \tag{7}$$

we obtain the desired relation between h_1, K_1/K_3, K_2/K_1 and γ or ψ, valid at the stability limit of the undistorted state for the onset of a periodic distortion. When solving Eq. (7), the value of N_1 was adjusted so that increasing it did not produce any changes above an error limit $\leq$2.5% in the determined relation between h_1, K_1/K_3, K_2/K_1 and γ or ψ. As was seen previously [10] in pre-tilted nematic slabs (occurring in geometries I and II) the periodic distorted state may be reached on increasing the magnetic field from the undistorted state either directly as given by 7 or by a different path through the homogeneously distorted state as an intermediate state, which results from the undistorted state at h = 1 on increasing the magnetic field, but is then unstable against the onset of a periodic distortion. At the stability limit of the homogeneously distorted state against the onset of a periodic distortion the determinant of the stability matrix (6) evaluated in the homogeneously distorted state goes to zero. The selected wave vector $\vec{q}$ of the periodic distortion minimises $|S_{ij}|$ and as before from

$$|S_{ij}|_{\min}(h_2, K_1/K_3, K_2/K_1, \gamma) = 0 \tag{8}$$

we obtain the relation between h_2, K_1/K_3, K_2/K_1 and γ valid at the stability limit of the homogeneously distorted state for the onset of a periodic distortion. To determine the stability matrix in the homogeneously distorted state it is necessary to find the unperturbed director field in this state. This was accomplished by minimisation of the Frank free energy plus the magnetic contribution in the unperturbed director amplitudes θ_{0j} and ϕ_{0j} using a conjugate gradients method [13] and considering a value for N_0 such that increasing it by 2 would leave the value of the minimised free energy unaffected within 1%. When solving Eq. (8) the value of N_1 was adjusted so that increasing it did not produce any changes above an error limit $\leq 2.5\%$ in the determined relation between h_2, K_1/K_3, K_2/K_1 and γ.

3. RESULTS

Depending on the values of h_1 and h_2 different behaviours are possible on increasing the magnetic field; when $h_1 < 1$ the undistorted state (US) looses stability directly to a periodic distorted state (PDS) at $h = h_1$. When $h_1 > 1$ US looses stability to the homogeneously distorted state (HDS) at $h = 1$ (the usual Fréedericksz transition). At $h = h_2$ HDS looses stability to PDS. In Figures 2 and 3 relations 7 and 8 are graphed as K_2/K_1 versus K_1/K_3 for $h = 1$ and different values of the pre-tilt angle γ for geometries of type I and type II respectively. As the graphics of the relations 7 and 8 were obtained for $h = 1$, the lines plotted separate regions of different behaviour. In region A at $h = 1$ the US looses stability to the HDS. In sub-region A_1 the transition US-HDS is continuous while in sub-region A_2 it is discontinuous, since in this sub-region for $h = 1$ a minimum of F_a with $F_a < 0$ already exists. The dashed line separating the two sub-regions is a line of tricritical points. In region B at $h = 1$ a minimum of F_a with $F_a < 0$ already exists and the US looses stability to the HDS that in turn is also unstable relatively to a PDS. In region C the US looses stability directly to a PDS at some value of $h = h_1 < 1$. In Figure 4 the results for geometries of type III are shown, relation 7 is independent of K_3 and is graphed as ψ versus K_2/K_1 for $h=1$. The absence of pre-tilt excludes Region B. In Figure 5 the connection between geometries I and II close to the pure bend geometry is established.

The global features of the phase diagrams for geometries of type I, II and III shown in Figures 2, 3 and 4 can be addressed on the basis of the mechanisms identified by Lonberg and Meyer[2] and Allender *et al.* [5] favouring the occurrence of periodic distortions in the pure splay and bend geometries respectively. In the pure splay geometry and close to it, type III geometry for small ψ, when $K_1 > K_2$ splay avoidance is achieved through the PDS (region C) as in [2]; for ψ close to $\pi/2$ when $K_1 < K_2$ the PDS avoids the twist [4]. In type II geometries for low γ values (close to splay geometry) and when $K_1 > K_2$ again PDS avoids splay (region C), for γ closer to $\pi/2$ the bend geometry is approached and when $K_3 > K_1 \geq K_2$ PDS avoids bend but PDS cannot be reached directly from the US and so it is a B type region [5]. In type I geometries for low γ values (close to twist geometry), and when $K_2 > K_1$ again PDS avoids twist (region C) [4]. For γ closer to $\pi/2$ the bend geometry is approached and a situation similar to type II geometries is found, with the important difference that in type I geometries the A_2 region inside which the B region can appear is limited to a fraction of the

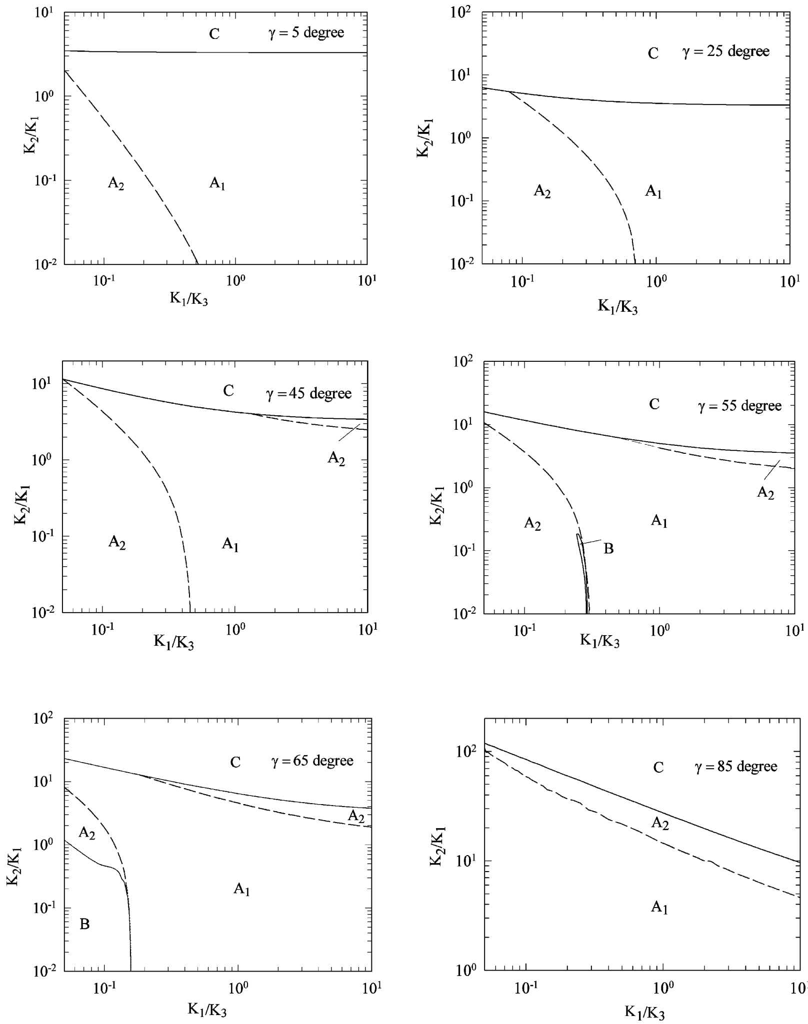

FIGURE 2 Diagrams defining in the K_1/K_3, K_2/K_1 plane the ranges of onset of the different states for the intermediate geometries of type I. In A US looses stability to HDS at $h = 1$. In A_1 the transition US-HDS is continuous while in A_2 it is discontinuous. In B at $h = 1$ the US looses stability to the HDS that in turn is unstable against the formation of PDS at the same field $h = 1$. In C US looses stability directly to PDS at $h = h_1 < 1$.

total A region. The determination of the director field in the PDS for the B and C regions should be done before a more detailed discussion of the phase diagrams for intermediate γ values can be carried out, but that

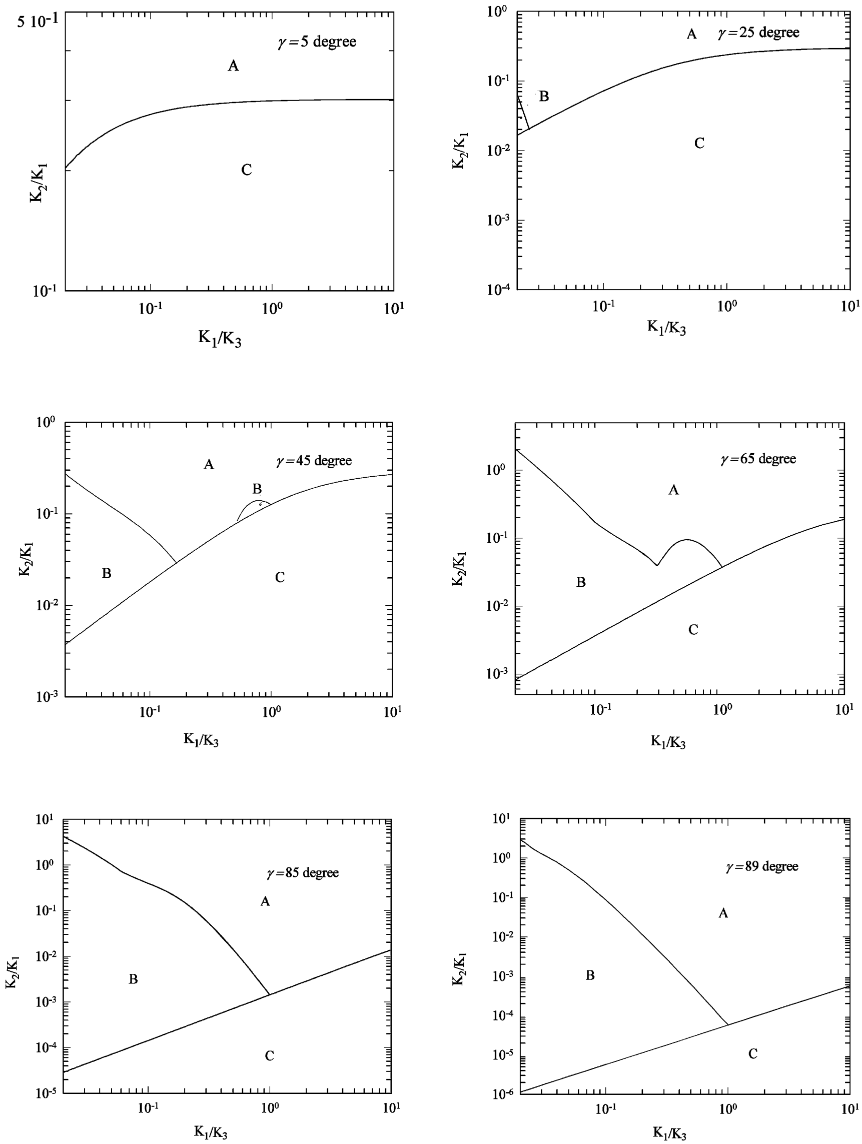

FIGURE 3 Diagrams defining in the K_1/K_3, K_2/K_1 plane the ranges of onset of the different states for the intermediate geometries of type II. Region A is of A_2 type except for $K_1 = K_3$ where it is of A_1 type.

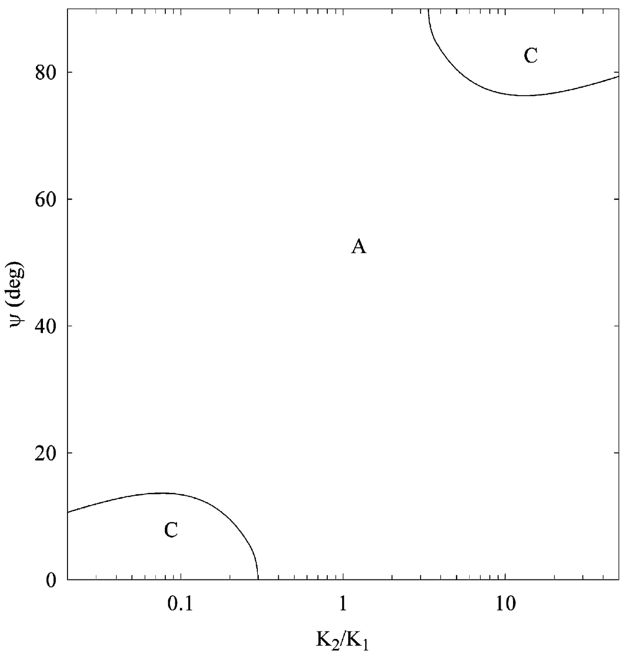

FIGURE 4 Diagrams defining in the ψ, K_2/K_1 plane the ranges of onset of the different states for the intermediate geometries of type III. Region A is of A_1 type.

determination is not performed in a stability analysis study and so it is out of the scope of this work.

The range of elastic constants studied is worth a word of explanation; while $K_1/K_3 < 1$ is expected for rod-like nematic low molecular weight liquid crystals (LMWLC) [11,15], $K_1/K_3 > 1$ is expected for semi-flexible liquid crystal polymers (PLC) [16]. $K_2/K_1 < 1$ is expected both for LMWLC and PLC [11,15], and this anisotropy is predicted to increase as the molecular weight or the concentration increases [16]. But near a nematic-smectic transition K_2 diverges and K_1 stays approximately constant [15] and so $K_2/K_1 >> 1$ is physically possible (corresponding to region C in Fig. 2).

4. CONCLUSION

We found that in pre-tilted nematics with sufficiently high elastic anisotropy the homogeneous distorted state (HDS) appearing above the magnetic field driven Fréedericksz transition may be replaced by a periodic distorted state (PDS). The transitions between the different states are

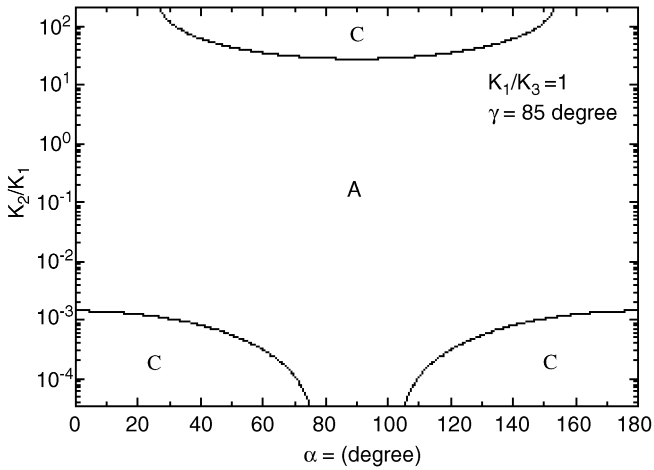

FIGURE 5 Diagram defining in the α, K_2/K_1 plane the ranges of onset of the different states as obtained from relation 7 with $K_1/K_3 = 1$ and $\gamma = 85$ degree. $\alpha = \pi/2$ is geometry I, $\alpha = \pi$ is geometry II.

not continuous in general. For a particular range of the elastic constants ratios K_1/K_3, K_2/K_1 and the pre-tilt angle γ, the periodic distorted state that appears at $h = 1$ is not reached directly but through the homogeneously distorted state. The transition undistorted state-homogeneously distorted state may be either continuous or discontinuous as found in pre-tilted nematics in other Fréedericksz transition geometries [10,14,17,18]. In type III geometries only regions A_1 and C are found.

REFERENCES

[1] Cladis, P. & Torza, S. (1975). *J. Appl. Phys.*, *46*, 584.
[2] Lonberg, F. & Meyer, R. B. (1985). *Phys. Rev. Lett.*, *55*, 718.
[3] Chu, K. C. & McMillan, W. L. (1977). *Phys. Rev. A*, *15*, 337.
[4] Kini, U. D. (1986). *J. Physique*, *47*, 693.
[5] Allender, D. W., Hornreich, R. M., & Johnson, D. L. (1987). *Phys. Rev. Lett.*, *59*, 2654.
[6] Kini, U. D. (1990). *Liquid Crystals*, *7*, 185.
[7] Kini, U. D. (1994). *Liquid Crystals*, *17*, 65.
[8] Kini, U. D. (1996). *Mol. Cryst. Liq. Cryst.*, *289*, 181.
[9] Casquilho, J. P., Gonçalves, L. N., & Figueirinhas, J. L. (1998). *Phys. Rev. E*, *58*, 626.
[10] Figueirinhas, J. L., Gonçalves, L. N., & Casquilho, J. P. (1999). *Phys. Rev. E*, *60*, 2985.
[11] De Gennes, P. G. & Prost, J. (1993). *The Phy. of Liq. Crystals* (Oxford: Clarendon).
[12] Fischer, F. (1976). *Z. Naturforsch, 31a*, 302; Nehring, J. (1979). *Phys. Lett., 72A*, 446; Deuling, H. J., Gabay, M., Guyon, E., & Pieranski, P. (1975). *J. Physique*, *36*, 689.
[13] Press, W., Flannery, B., Teukolsky, S., & Vetterling, W. (1990). *Numerical Recipes*, (Cambridge: Cambridge University Press).

[14] Onnagawa, H. & Miyashita, K. (1974). *Jap. J. Appl. Phys.*, *13*, 1741.
[15] Chandrasekhar, S. (1992). *Liquid Crystals*, 2nd ed. (Cambridge: Camb. Univ. Press).
[16] Taratuta, V. G., Lonberg, F., & Meyer, R. B. (1988). *Phys. Rev. A, 37*, 5, 1831; Lee, S. D. & Meyer, R. B. (1988). *Phys. Rev. Lett.*, *61*, 19, 2217.
[17] Motooka, T. & Fukuhara, A. (1979). *J. Appl. Phys.*, *50*, 3322.
[18] Yamada, H. (1984). *Mol. Cryst. Liq. Cryst.*, *108*, 93.