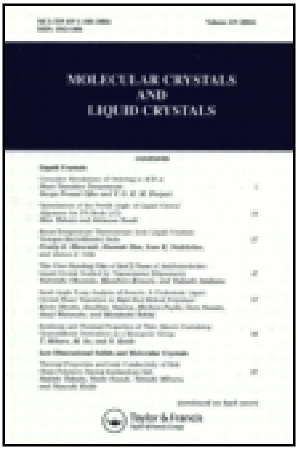

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On Certain Liquid Crystal Defects in a Magnetic Field

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On Certain Liquid Crystal Defects in a Magnetic Field

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We find some interesting defect configurations in nematic, smectic and discotic liquid crystals in the presence of a magnetic field. We consider both positive and negative anisotropy materials subjected to a uniform or an all circular magnetic field. We have undertaken an energy analysis of many of these configurations.

Keywords: Defects, Disclinations, Dislocations, Defects in Magnetic Fields

INTRODUCTION

In a magnetic field a liquid crystal exhibits many interesting defect configurations arising due to the diamagnetic anisotropy of the molecules. The structure and properties of these defects have been studied in detail in nematics.[1–5] But there does not appear to be such a thorough investigation in smectics and discotics. In this paper we look at some of the possible defect states in nematics, smectics and discotics in the presence of a magnetic field. We have considered not only the effect of a uniform magnetic field but also that of an all circular field generated by a linear current element. In addition we have treated the cases of positive as well as negative diamagnetic anisotropy.

Some interesting new results have emerged. For example, in nematics we find a new interaction law between disclinations when a uniform magnetic field is applied normal to the disclination lines. They interact with a distance independent force. A method of generating Poincaré half defects has been suggested. We also find that bubble domains can exist as natural states in an all circular magnetic field. In smectic A we find that screw dislocations in the presence of a uniform magnetic field interact like crystal screw dislocations. There also appears a structural instability resulting in screw dislocations in the presence of a magnetic field. The $s = +1$ all radial configuration develops a spiral dislocation in an all circular field above a threshold. In smectic C, however, we find a dispiration under a similar field. In columnar discotics, in addition to the smectic like spiral distortion we also get a helical columnar configuration in an all circular field.

NEMATICS

Interaction between disclinations

When a magnetic field is applied normal to an half integral disclination line the resultant structure is a planar soliton terminating in a $\pm 1/2$ disclination.[3] Interaction between two such defects is considered below.

Consider two $^{1/2}$ wedge disclinations of opposite sign separated by a large distance. The splay soliton obtained in a magnetic field H acting perpendicular to the line connecting them is shown in Figure 1(a). Here in the absence of the field the director at large distances is perpendicular to the line connecting the defects. It is

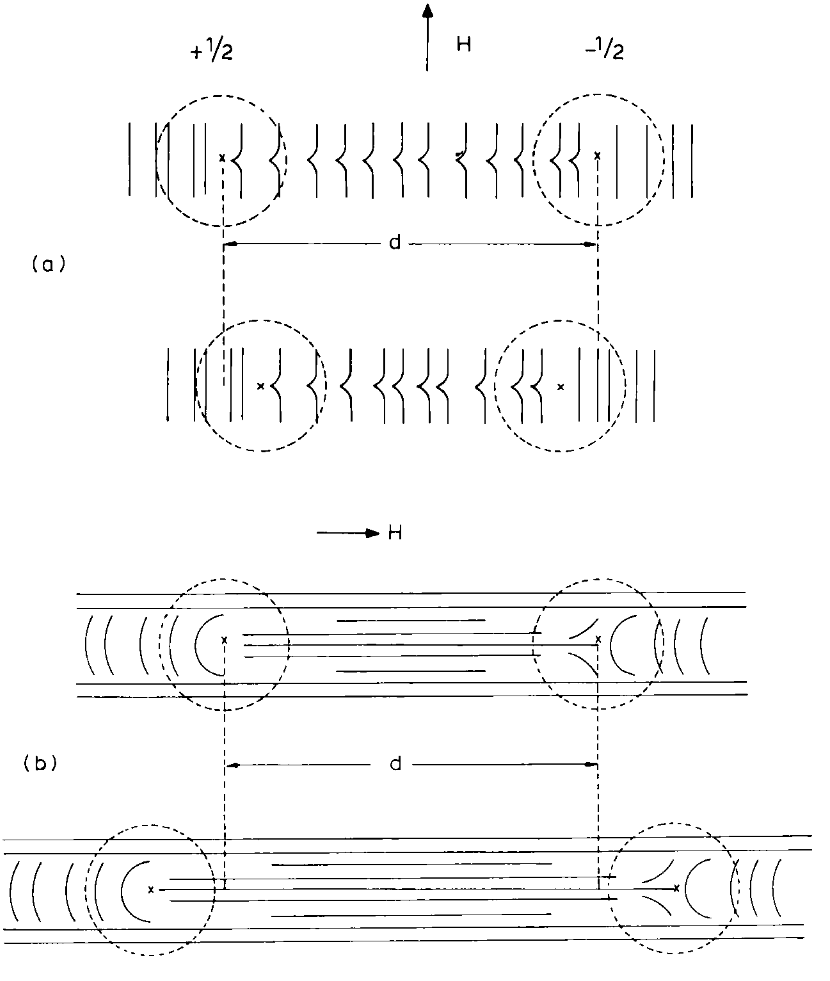

FIGURE 1 A pair of unlike disclinations of strength 1/2 in a magnetic field acting normal to the disclinations lines (a) Field perpendicular to the line joining the disclinations, (b) Field along the line joining disclinations.

clear from the figure that most of the splay distortion is confined to the region between the disclinations and within the width of the soliton. We see that by moving the two disclinations towards each other the director distortion in the regions indicated by dashed circles (with the radii of the order of magnetic coherence length) and in the far off regions are not much affected. But this process reduces the energy of the configuration in the central region. To a good approximation this is $\Delta E = 2H\,(k\chi_a)_{1/2}\,\Delta d$, with χ_a as the diamagnetic anisotropy and k as the elastic constant in the one constant approximation. This is proportional to the change Δd in the distance of separation between the disclinations. Hence we find a distance independent force as opposed to the familiar $1/d$ law.

Interestingly, unlike disclinations can also repel one another under certain conditions. This is depicted in Figure 1(b). Here the magnetic field is parallel to the line joining the disclinations. We get planar bend soliton going on either side to infinity away from the defects. The distortion in the region indicated by the dashed circles is again unaltered by changes in d. But in the central, nearly distortion-free region, energy decreases with increase of separation. Thus the field favours repulsion. The change in energy in this case is

$$\Delta E = -\frac{\chi_a H^2}{2}\,\Delta d.$$

Thus we see that two disclinations of opposite strength will attract or repel with a distance independent force. The magnitude of the attractive and repulsive forces are, however, different. In the same way interaction between like disclinations can also be repulsive or attractive with a force independent of distance of separation. The same arguments can be extended to twist disclinations as well.

It must be remarked that the standard elastic interaction between disclinations is not totally absent in the presence of the magnetic field. But exact calculation of the net interaction is not easy. What we can do is to undertake and approximate analysis. We know that the elastic free energy density varies as $k\,(\nabla\theta)^2$ [θ is the director orientation] where as the magnetic energy density varies as $\chi_a H^2 \sin^2\theta$. Hence over distances less than the coherence length $\xi = (k/\chi_a H^2)^{1/2}$, we can, to a good approximation ignore the magnetic term. Thus we can argue that when the separation d between the unlike (like) defects is much less than ξ the elastic attractive (repulsive) interaction dominates. The distance independent law is valied for $d >> \xi$. Therefore d of the order of ξ is probably the region where we go from the $1/d$ law to the distance independent law of interaction.

Poincaré structures

It is known[6,7] that a line singularity of strength ± 1 can end in a half disclination point. This implies that a line singularity can be terminated with an unlike pair of 1/2 disclination points. We suggest here a method of getting these defect states which appear not to have been seen experimentally so far.

If a magnetic field is applied parallel to the director of a homeotropically aligned nematic with negative diamagnetic anisotropy, it will undergo a Freedericksz transition at a critical field. The resulting structure will be non-singular as shown in Figure 2(a). But in a central region the director still is opposing the magnetic torque. Hence at fields much higher than this critical field this structure can break down to the one shown in Figure 2(b). Here a $s = +1$ line singularity has ended in a pair of unlike half Poincaré point singularities. This is the analogue of the pinching effect in Brochard Walls.

This phenomena can be expected in nematic discotics as they usually have negative diamagnetic anisotropy. In rod-like nematics it is easier to get systems with negative dielectric anisotropy. Here the above arguements are valid *mutatis mutandis* in the presence of an electric field.

Bubble domains

Symmetry of a nematic liquid crystal permits one to consider, in a uniform magnetic field, cylindrical shell structures or bubble domains[5] separating the inside and the outside regions by a 180° twist or bend distortion. We now investigate the possibility of such a bubble domain in the presence of an all circular magnetic field H_α =

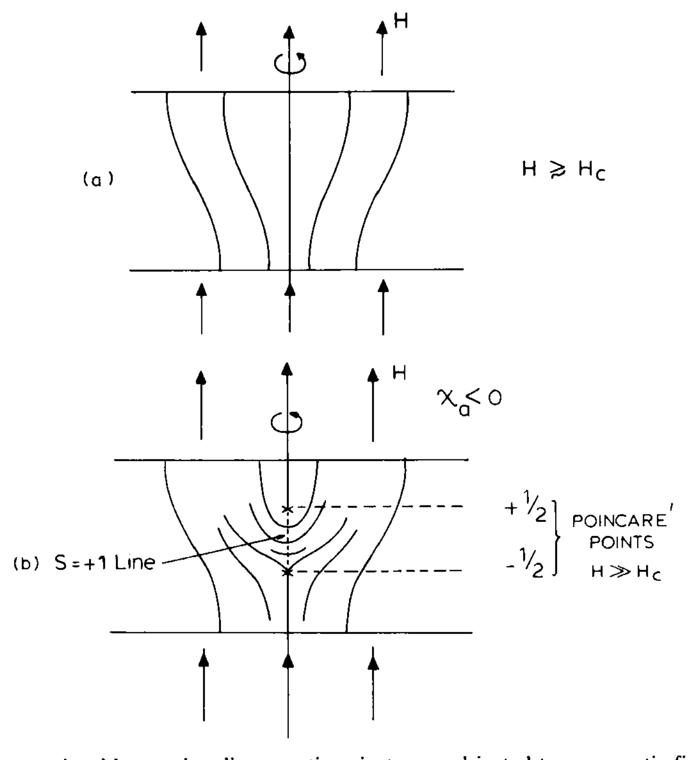

FIGURE 2 A nematic with negative diamagnetic anisotropy subjected to a magnetic field along the director, in the homeotropic geometry. (a) Just above the Freedricksz threshold. (b) At much higher fields.

A/r acting on a nematic with negative diamagnetic anisotropy. The director n defined in cylindrical polars are:

$$n = [\sin\theta\cos(\phi - \alpha), \quad \sin\theta\sin(\phi - \alpha), \quad \cos\theta]$$

The free energy density is given by

$$F = \frac{k}{2}[(\nabla\theta)^2 + \sin^2\theta(\nabla\phi)^2] + \frac{\chi_a A^2}{2r^2}\sin^2\theta\sin^2(\phi - \alpha)$$

The differential equation obtained by minimization of this free energy are

$$k[(\nabla^2\theta) - \sin\theta\cos\theta\,(\nabla\phi)^2] - \frac{\chi_a A^2}{r^2}\sin\theta\cos\theta\sin^2(\phi - \alpha) = 0$$

$$k(\nabla^2\phi) - \frac{\chi_a A^2}{r^2}\sin(\phi - \alpha)\cos(\phi - \alpha) = 0$$

The solutions satisfying the boundary conditions $\theta = 0$ at $r = 0$ and $\theta = \pi$ at $r = \infty$ are:

$$\theta = 2\tan^{-1}(r/r_o)^\eta \text{ and}$$

$$\phi = \alpha + \pi/2$$

where

$$\eta = [1 + \chi_a A^2/k]^{1/2}$$

Here r_o is the point at which θ becomes $\pi/2$. This represents a Bloch bubble domain as shown in Figure 3. The variation of θ with respect to r/r_o is shown in Figure 4 for different values of η. We see that the width of the domain wall decreases as the field increases. Thus in such a field a bubble domain is a natural soliton solution. The total energy of this structure per unit length is found to be $4\pi k\eta$. Interestingly the energy is independent of its radius r_o. At high fields $\eta \simeq [\chi_a A^2/k]^{1/2}$ and the energy is $4\pi A\,(k\chi_a)^{1/2}$, which is $2\pi r_o$ times the surface tension of the planar soliton obtained in uniform fields.

Bubble domains exist also in diamagnetically positive materials but here the field should be such that $\chi_a A^2 > k$. At lower fields we find a collapsed $+1$ all circular disclination.[8] This becomes a planar singular structure at the critical value of $A = (k/\chi_a)^{1/2}$. In this all circular planar structure we can now construct a twist-bubble

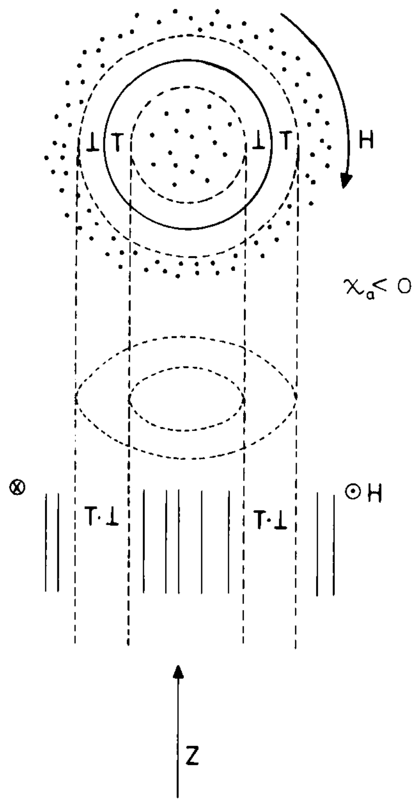

FIGURE 3 A twist-bubble domain in a nematic with $\chi_a < 0$, in an all circular field. The domain is bounded by the dashed contours.

or an inplanar bend-bubble domain. It is easy to analyze the twist-bubble where the boundary condition are

$$\text{at } r = 0 \;\; \theta = -\pi/2 \quad \text{and} \quad \text{at } r = \infty \;\; \theta = +\pi/2$$

from the equation of equibrium we get

$$\phi = \alpha + \pi/2$$

and $$\theta = 2 \tan^{-1} [r/r_o]^{\eta} - \pi/2$$

where $$\eta = [\chi_a A^2/k - 1]^{1/2}$$

and the extra energy due to the bubble domain is again $4\pi k\eta$ per unit length.

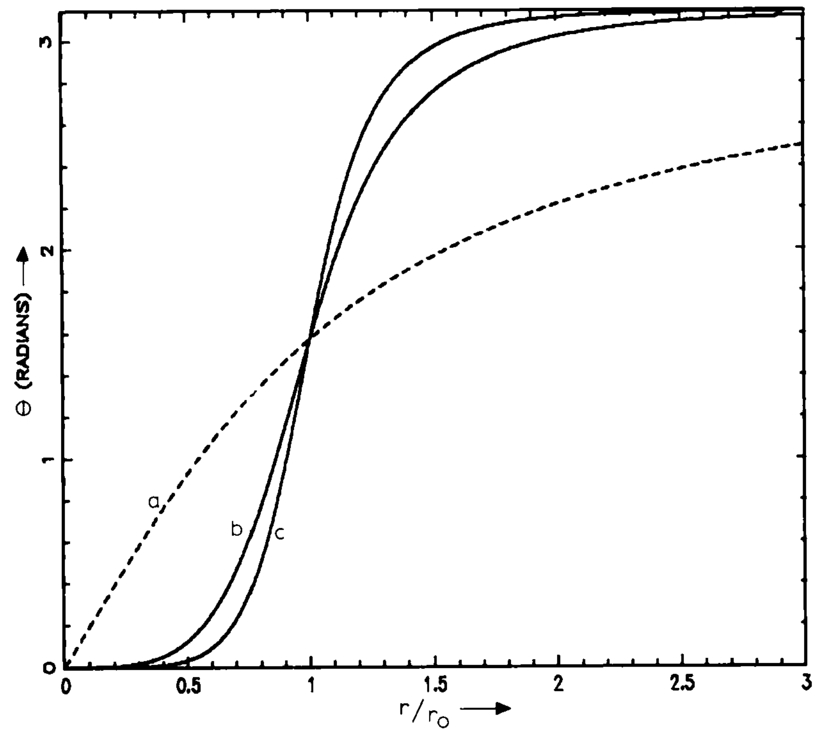

FIGURE 4 The director tilt θ in a twist-bubble domain of radius r_o, as a function of the distance from the centre. (a) In the absence of the field, i.e., $\eta = 1$. (b) In a field with $\eta = 4$ and (c) with $\eta = 6$.

SMECTICS

Interaction between screw dislocations in smectic A

In the linear elastic theory screw dislocations in smectic A have neither self energy nor do they interact. We shall consider this problem in a uniform field acting along z-axis. The free energy density for $\chi_a > 0$ is

$$F = \frac{B}{2}\left(\frac{\partial u}{\partial z}\right)^2 + \frac{k_{11}}{2}\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right]^2 + \frac{\chi_a H^2}{2}\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right]$$

where u = The layer displacement

B = The elastic constant for lattice dilation

k_{11} = the elastic constant for layer curvature

Minimization of energy results in the following equation of equilibrium:

$$B\left(\frac{\partial^2 u}{\partial z^2}\right) - k_{11}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]^2 u + \chi_a H^2\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right] = 0$$

This permits the following solution

$$u = \frac{b}{2\pi}\tan^{-1}(y/x)$$

This is the familiar screw dislocation. Its strength b is an integral multiple of a_o the layer spacing. This has an energy per unit length given by

$$E = \frac{b^2}{4\pi}\chi_a H^2 \ln(R/r_c)$$

Here R is the sample size and r_c is the core radius. This energy is purely magnetic with no elastic contribution whatever.

A linear combination of such solutions is also valid. This results in an interaction energy per unit length

$$E_i = \left(\frac{b_1 b_2}{2\pi}\right)\chi_a H^2 \ln(2R/d)$$

with d as the distance of separation between the dislocations.

Hence an interaction exists in a magnetic field. Like dislocations repel and unlike dislocations attract with a force proportional to $1/d$. This interaction is exactly the same as that between screw dislocations in crystals. The same interaction law is also obtained in a compressed smectic due to the non-linear term of the form

$$\frac{B}{2}\left(\frac{\partial u}{\partial z}\right)\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right].$$

Due to its similarities with the magnetic term we find the force to be proportional to the applied compressive strain. It may be mentioned in passing that a very similar interaction law has also been proposed by Pleiner,[9] again arising from a non-linearity but of a different nature. In his analysis the dislocations interact even in a stress-free smectic.

Field induced defects

(1) Hz field Consider a homeotropically aligned sample with negative diamagnetic anisotropy and with layers in the x-y plane. The free energy density in presence of a field parallel to z-axis, for small layer distortions u is given by

$$F = \frac{B}{2}\left(\frac{\partial u}{\partial z}\right)^2 + \frac{k_{11}}{2}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)^2 - \frac{\chi_a H^2}{2}\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right]$$

It can be easily verified that $u = \frac{b}{2\pi} \tan^{-1}(y/x)$ which represents a screw dislocation, is again a solution of the equation of equilibrium and the total energy per unit length is given by

$$E = -\frac{\chi_a H^2 b^2}{4\pi} \ln(R/r_c)$$

Since this energy is always negative the structure develops an instability through a proliferation of screw dislocations. Solutions with contributions from the elastic term will be of higher energy and a threshold will be needed to excite them.

We can expect the same solution in the case of materials with negative dielectric anisotropy, in the presence of an electric field along the layer normal.

(2) H_α field Here we will investigate the same geometry as in (1) but with $\chi_a > 0$ and in the presence of an all circular field acting parallel to the layers. We expect a perturbation of the form

$$n_r = 0, \quad n_\alpha = \frac{-1}{r}\left(\frac{\partial u}{\partial \alpha}\right), \quad n_z = 1 - \frac{1}{2r^2}(\partial u/\partial \alpha)^2$$

The free energy density can be written as

$$F = \frac{k_{11}}{2r^4}\left(\frac{\partial^2 u}{\partial \alpha^2}\right)^2 - \frac{\chi_a A^2}{2r^4}\left(\frac{\partial u}{\partial \alpha}\right)^2$$

Minimization gives

$$\frac{k_{11}}{r^4}\frac{\partial^4 u}{\partial \alpha^4} + \frac{\chi_a A^2}{r^4}\frac{\partial^2 u}{\partial \alpha^2} = 0$$

This permits again the screw dislocation solution $u = b/2\pi\, \alpha$ which has an energy per unit length, given by

$$E = -\frac{\chi_a A^2 b^2}{8\pi}\left[\frac{1}{r_c^2} - \frac{1}{R^2}\right]$$

As $R > r_c$ this energy is always negative. Hence the system is again destabilised through screw dislocation creation. This screw dislocation is different from the classical one in the sense that its enrgy is finite even for an infinite sample.

Spiral instability in H_α field

Consider the wedge +1 disclination along the z axis with an all radial director configuration. In an all circular magnetic field of the form $(0, A/r, 0)$ acting parallel to the smectic layers with molecules having positive diamagnetic anisotropy we can expect a perturbation of the form

$$n_r = 1 - \frac{1}{2r^2}\left(\frac{\partial u}{\partial \alpha}\right)^2, \quad n_\alpha = -\frac{1}{r}\left(\frac{\partial u}{\partial \alpha}\right), \quad n_z = 0$$

Here u is the layer displacement along the radial direction. The free energy density upto second order in u is given by

$$F = \frac{k_{11}}{2}\left[\frac{1}{r^2} + \frac{1}{r^4}\left(\frac{\partial u}{\partial \alpha}\right)^2\right] - \frac{\chi_a A^2}{2r^2}\left[\frac{-1}{r}\frac{\partial u}{\partial \alpha}\right]^2$$

minimisation of the free energy gives the solution

$$u = \frac{a_o N}{2\pi}\alpha$$

where a_o is the layer spacing and the N an integer. This represents a spiral distortion, resulting in a helical wrapping of smectic layers. The change in free energy due to this distortion is

$$\delta F = [k_{11} - \chi_a A^2]\frac{1}{2r^4}\left(\frac{\partial u}{\partial \alpha}\right)^2$$

Thus, for values of A greater than $(k_{11}/\chi_a)^{1/2}$ the system is unstable against such distortions. Such a structure was first discribed by Kleman and Parodi.[10] This is a kind of dislocation. As indicated by them this structure can even have a weak twist in the z-direction. This solution is very different from the spiral structures discussed by Bouligand[11] for smectic A with layers ending on a cylindrical boundary.

Smectic C

In a magnetic field H_z acting normal to the layers and with only layer displacements we find again the same solutions as those obtained earlier for smectic A. However, in a field (O, H_α, O) acting parallel to the smectic layer, we get a different solution. Here we can get as in smectic A a screw dislocation. In addition even a disclination in the C -director can be expected. For a small perturbation u, the free enrgey density with $\chi_a > 0$ becomes

$$F = \frac{k}{2}\theta^2(\nabla\phi)^2 - \frac{\chi_a A^2}{2r^2}\left[\frac{1}{r}(\partial u/\partial\alpha) + \theta\sin(\phi - \alpha)\right]^2 + \frac{k_{11}}{2r^4}\left[\frac{\partial^2 u}{\partial\alpha^2}\right]^2$$

where u = layer displacement

θ = tilt angle

ϕ = azimuth of the C director

k = the elastic constant for bend or splay in the C-director

Minimization yields solution:

the disclination $\phi = \alpha + \pi/2$ and

the screw dislocation $u = a_o N/2\pi\ \alpha$

The free energy density for this solution is

$$F = \frac{\theta^2}{2r^2}[k - \chi_a A^2] - \frac{\chi_a A^2}{2r^2}\left[\left(\frac{b}{2\pi r}\right)^2 + \frac{b\theta}{2\pi r}\right]$$

The system will have a negative energy due to the screw dislocation alone. At fields higher than the critical field $A_c = (k/\chi_a)^{1/2}$ this energy is further lowered by the creation of a disclination in the C director. The resultant distortion has both dislocation and disclination characteristics. In other words we end up with a dispiration as the low energy defect for field $A > A_c$.

COLUMNAR DISCOTICS

The simplest of the columnar discotics has hexagonal symmetry. One possible defect state has columns bent around the z-axis into concentric circles,[11] i.e., $n_\alpha = 1$. In an all circular field with $\chi_a < 0$ (this is usually the case for discotics) this defect state gets perturbed. We can assume the perturbation to be of the form:

$$n_r = -\frac{1}{r}\left(\frac{\partial u}{\partial\alpha}\right), \quad n_\alpha = 1 - \frac{1}{2r^2}\left(\frac{\partial u}{\partial\alpha}\right)^2, \quad n_z = 0$$

where u is the displacement of the columns perpendicular to the director $\mathbf{n}$. The various columnar circles in any given plane get interconnected to form a spiral. The change in free energy density due to this distortion is

$$\delta F = \frac{1}{2r^4}\left(\frac{\partial u}{\partial \alpha}\right)^2 (k_{33} - \chi_a A^2)$$

k_{33} = The bend elastic constant
Here to a good approximation we can neglect the lattice distortions. the minimisation of the free energy permits the solution in $u = (b_\perp/2\pi)\alpha$, where $b_\perp$ is an integral multiple of the spacing of the columns perpendicular to the z-axis. This will exist above a threshold given by $A_c = [k_{33}/\chi_a]^{1/2}$. Thus a smectic-like spiral dislocation exists in addition to the disclination in the director n. We have a dispiration configuration in which a classical disclination is associated with a spiral dislocation.

Another possible mode of distortion in the same field is of the form

$$n_r = 0, \quad n_\alpha = 1 - \frac{1}{2r^2}\left(\frac{\partial u}{\partial \alpha}\right)^2, \quad n_z = -\frac{1}{r}\left(\frac{\partial u}{\partial \alpha}\right)$$

Here also neglecting the lattice distortions we can write the extra free energy density as

$$\delta F = \frac{1}{2r^4}\left(\frac{\partial u}{\partial \alpha}\right)^2 (2k_{33} - \chi_a A^2)$$

The critical field here is $A_c = [2k_{33}/\chi_a]^{1/2}$, above which we get $u = (b_\parallel/2\pi)\alpha$. Here $b_\parallel$ is an integral multiple of the layer spacing parallel to z-axis. This results in a helical connection between the circular column, i.e., we get coaxial helices.

These two possible modes are very different from the spiral columns around cylinder and a helical distortion around a helix proposed by Kleman[12] and Bouligand[11] for columnar discotics, from the theory of developable domains.

SPECULATIONS ON THE CORE NEAR A-C TRANSITION

Consider a ± 1 disclination in smectic C near A-C transition. Very near the transition point the order parameter θ is small. Using the Landau theory of A-C transition, we get the Ginsburg-Pitaevskii equation for the core in the presence of a H_z field for $\chi_a > 0$.

$$1/\xi \frac{\partial}{\partial \xi}\left(\xi \frac{\partial f}{\partial \xi}\right) - f/\xi^2 + f(1 - f^2) = 0$$

where

$$\xi = r/\xi_o, \ \xi_o = (-k/\alpha')^{1/2}$$

$$f = \theta/\theta_o \quad \theta_o = \text{Tilt angle at } r \rightarrow \infty = (\alpha'/\beta')^{1/2}$$

$$\alpha' = \alpha + \chi_a H^2 \quad \beta' = \beta - \frac{2}{3}\chi_a H^2$$

$$\alpha = \alpha_o(T - T_c) \quad \beta > 0$$

α_o and β are thermodynamic parameters of the classical Landau expansion. For $\beta' > 0$ the tilt angle drops to zero at the centre of the singularity. Most of the variation in θ takes place over a distance ξ_o. As H increases ξ_o increases slowly sweeping whole area. At the critical field $H = [|\alpha|/\chi_a]^{1/2}$ tilt angle becomes zero every where, i.e., we get a smectic A state.

It is possible for β' to be negative depending on the thermodynamic parameter β and the field strength H. When this happens we can speculate on the possibility of a first order transition to the smectic A state.

On the smectic A side of the A-C transition with $\chi_a > 0$ and an all circular field acting parallel to the smectic layers the free energy density is

$$F = \frac{k}{2}[(\nabla\theta)^2 + \theta^2/r^2] + \frac{\alpha\theta^2}{2} + \frac{\beta\theta^4}{2} + \frac{\chi_a A^2}{2r^4}(1 - \theta^2 + \theta^4/3)$$

From this we conclude that the coefficient of θ^2 (which is always positive in the absence of the field) has a fair chance of becoming negative at very small distances. Within this range we get a smectic C-like disclination. A detailed analysis of this again leads to a Ginsburg-Pitaevskii type equation.

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