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# Determining the anchoring strength in a capillary using topological defects

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We consider a smectic A* phase in a capillary with surface anchoring that favours parallel alignment. If the bulk phase of the smectic is the standard twist-grain-boundary phase of chiral smectics, then there will be a critical radius below which the smectic will not have any topological defects. Above this radius a single screw dislocation in the centre of the capillary will be favoured. Along with surface anchoring, a magnetic field will also suppress the formation of a screw dislocation. In this note, we calculate the critical field at which a defect is energetically preferred as a function of the surface anchoring strength and the capillary radius. Experiments at a few different radii could thus determine the anchoring strength.



## 1. Introduction

Boundary conditions play an essential role in liquid crystal physics and they cannot be taken with a cavalier attitude. Even if the boundary is very far away, surface effects in liquid crystals can be very important because of typically long-range, algebraic correlations in these soft materials. Indeed, in device applications one is often interested in the surface effects on bulk ordering: such effects are a key element in the twisted nematic display [1].

In this note we consider a smectic liquid crystal which, in bulk, would form a Renn–Lubensky [2] twist-grain-boundary (TGB) phase [3]. We will show that if this smectic is confined to the classic capillary geometry [4, 5] with the layer normals parallel to the capillary axis then for sufficiently small radii an undefected smectic A phase persists while for larger radii screw dislocations can enter as shown in figure 1. While this, in principle, can give a very clean determination of the anchoring strength $W$ it is rather impractical to do an experiment on a sequence of capillaries with small differences in their radial size. Instead, we show how the imposition of a magnetic field also suppresses defect formation. In this case, at fixed radii, the applied field may be scanned and the critical field may be determined. Doing this measurement at a few radii should make it possible to determine $W$.

## 2. Results

We start with the free energy of a smectic confined to a region $\Omega$ in the $xy$ plane, and assume that the capillary is infinite in the $z$ direction. We further assume there is an infinite energy cost for the director to have a radial component at the surface. The appropriate free energy to quadratic order is then [6]

$$\begin{aligned} F &= F_{\text{bulk}} + F_{\text{surface}} \\ &= \int \mathrm{d}z \int_{\Omega} \mathrm{d}^2x \left\{ \frac{B}{2}(\nabla_\perp u + \delta\mathbf{n})^2 + \frac{B_z}{2}(\partial_z u)^2 \right. \\ &\quad + \frac{K_1}{2}(\nabla_\perp \cdot \delta\mathbf{n})^2 + \frac{K_2}{2}(\nabla_\perp \times \delta\mathbf{n})^2 \\ &\quad \left. + \frac{K_3}{2}(\partial_z \delta\mathbf{n})^2 - \frac{\chi}{2}(\mathbf{H}\cdot\mathbf{n})^2 \right\} \\ &\quad - \int \mathrm{d}z \left\{ \int_{\partial\Omega} \mathrm{d}l \left[ K_2 q_0 \delta\mathbf{n}\cdot\mathbf{T} \right.\right. \\ &\quad \left.\left. + \frac{K_{24}}{2}\mathbf{N}\cdot[\mathbf{n}(\nabla\cdot\mathbf{n}) - (\mathbf{n}\cdot\nabla)\mathbf{n}] \right] \right. \\ &\quad \left. - \int_{\partial_+\Omega} \mathrm{d}l \left[ \frac{W}{2}(\mathbf{n}_\phi)^2 \right] \right\}. \end{aligned} \tag{1}$$

$\partial\Omega$ denotes the total boundary of the smectic region, including any boundaries at defects, while $\partial_+\Omega$ includes only the boundary with the capillary; $\mathbf{N}$ is the (outward pointing) normal to the surface and $\mathbf{T}$ is the surface tangent perpendicular to $\hat{z}$. The smectic order parameter is $\psi = |\psi| e^{i2\pi(z+u)/a}$, and thus the phase of the mass-density wave is $u$. The molecular director is $\mathbf{n} = \hat{z}(1-\delta n^2)^{1/2} + \delta\mathbf{n}$ with $\hat{z}\cdot\delta\mathbf{n} = 0$. The $K_i$ are the Frank elastic constants, $B$ and $B_z$ are proportional to the

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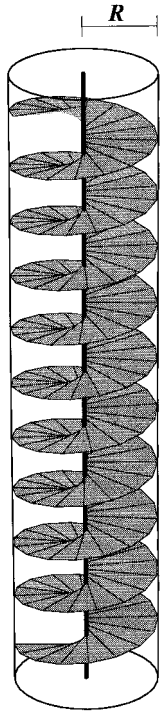


Figure 1. Screw dislocation in a capillary geometry. The dark centre line is the screw dislocation.



smectic order parameter squared $|\psi|^2$, $K_{24}$ is the saddle–splay elastic constant [7], $q_0$ is the equilibrium cholesteric pitch, $\chi$ is the negative diamagnetic susceptibility, $\mathbf{H} = H\hat{z}$ is a magnetic field, and $W$ is the anchoring strength which we want to determine. In (1) we have used the fact that the chiral bulk term $K_2 q_0 \nabla_\perp \times \delta\mathbf{n}$ can be rewritten as a surface term. While we are not explicitly interested in the saddle–splay term, there is no way to remove it from the problem—when there is a surface it must be included [8, 5]. It too serves to promote or hinder the formation of a central screw dislocation.

We note by symmetry along $\hat{z}$ that the problem can be reduced to a *two-dimensional* problem and thus the fields will have no $z$ dependence. The field configurations which minimize the bulk free energy satisfy the Euler–Lagrange equations:

$$0 = \nabla_\perp^2 u + \nabla_\perp \cdot \delta\mathbf{n} \qquad \text{and} \tag{2a}$$

$$0 = B(\nabla_\perp u + \delta\mathbf{n}) + \chi H^2 \delta\mathbf{n} - K_1 \nabla_\perp \nabla_\perp \cdot \delta\mathbf{n} - K_2(\nabla_\perp^2 \delta\mathbf{n} - \nabla_\perp \nabla_\perp \cdot \delta\mathbf{n}). \tag{2b}$$

The saddle–splay term can lead to a buckling instability toward a configuration with a non-zero divergence of $\delta\mathbf{n}$. In this note we will limit our attention to the effect of the anchoring term on defect formation; in our quadratic approximation the transverse distortions due to the defect decouple from the longitudinal distortions due to buckling. We will therefore assume $\nabla_\perp \cdot \delta\mathbf{n} = 0$. It would be an interesting extension of this work to study the nonlinear theory to understand buckling and its interplay with defects (cf. [9]).

We write this constraint in cylindrical coordinates as

$$\frac{1}{\rho}\partial_\rho(\rho \delta n_\rho) + \frac{1}{\rho}\partial_\phi \delta n_\phi = 0. \tag{3}$$

Using rotational invariance, we can assume that the nematic field $\delta\mathbf{n}$ is independent of $\phi$. In this case (3) implies that $\rho\delta n_\rho$ is constant. Since $\delta n$ must be well defined everywhere, including $\rho = 0$, the constant must be 0. Therefore $\delta\mathbf{n} = \delta n_\phi(\rho)\hat{\phi}$.

To find the minimum energy solution we must take into account the boundary terms. The outer surface energy in (1) may be expanded up to quadratic order in $\delta\mathbf{n}$:

$$F_{\text{surface}} = \int \mathrm{d}z \int_{\partial_+\Omega} \mathrm{d}l [\delta n_\phi(R)]^2 \left[\frac{W}{2} - \frac{K_{24}}{2R}\right] - K_2 q_0 \int \mathrm{d}z \int_{\partial_+\Omega} \mathrm{d}l\, \delta n_\phi(R), \tag{4}$$

where $R$ is the capillary radius. We work in the type II [6] limit in which the twist penetration depth $\lambda_0 = (K_2/B)^{1/2}$ is much bigger than the coherence length $\xi$; in this limit the contribution of the inner boundary terms turns out to be subleading. We may now calculate the minimum bulk energy for fixed $\delta n_\phi(R)$ and get an effective free energy $F(\delta n_\phi(R))$ which we may finally minimize over the number $\delta n_\phi(R)$. At this point we identify the *magnetic* twist penetration depth $\lambda_H^2 = K_2/(B + \chi H^2)$. We can solve (2) by introducing $\mathbf{Q} = \delta\mathbf{n} + (\lambda_H^2/\lambda_0^2)\nabla_\perp u$ [1] so that

$$\nabla_\perp^2 \mathbf{Q} - \frac{1}{\lambda_H^2}\mathbf{Q} = 0. \tag{5}$$

Note that (2*b*) implies that $u$ is independent of $\rho$ and thus $\mathbf{Q}$ only has components in the $\phi$ direction. In cylindrical coordinates (5) reduces to Bessel's modified equation with index $\nu = 1$ and so

$$Q_\phi(\rho) = C_1 K_1(\rho/\lambda_H) + C_2 I_1(\rho/\lambda_H). \tag{6}$$

We determine $C_1$ by insisting that $\delta\mathbf{n}$ be regular at the origin. The origin is, in fact, the *other boundary*. In particular, we might consider the possibility that there is a defect at the centre of the capillary. Recall that a screw dislocation is a layer configuration in which $u = am\phi/(2\pi)$ where $a$ is the layer spacing and $m$ is an integer. Note that since $u$ is independent of $\rho$, $u = am\phi/(2\pi)$ is the most general solution of the equations of equilibrium with $\nabla_\perp \cdot \delta\mathbf{n} = 0$. This implies that $\nabla_\perp u = \hat{\phi} am/(2\pi\rho)$ and is thus singular at the origin. Since $I_1(0) = 0$, we have,

near $\rho = 0$

$$\rho \delta n_\phi(0) + \frac{\lambda_H^2}{\lambda_0^2}\frac{am}{2\pi} = C_1 \lambda_H, \tag{7}$$

and so $C_1 = am\lambda_H/(2\pi\lambda_0^2)$. Thus the only free parameter in the bulk free energy is $C_2$ which is determined by demanding $\delta n_\phi(R) \equiv \delta n_0$:

$$C_2 = \frac{\delta n_0 + am\lambda_H/(2\pi\lambda_0^2)[(\lambda_H/R) - K_1(R/\lambda_H)]}{I_1(R/\lambda_H)}. \tag{8}$$

Taking the core size to be $\xi$ and working in the regime where $R \gg \lambda_0$, $\lambda_H \gg \xi$ we find that the bulk strain energy to leading order in $\lambda_H/R$ is

$$\begin{aligned} F_{\text{bulk}}(\delta n_0)/L \approx m^2 E_{\text{core}} &+ \chi H^2 \frac{a^2 m^2 \lambda_H^2}{4\pi\lambda_0^2}\ln(R/\xi) \\ &+ K_2 \frac{a^2 m^2 \lambda_H^2}{4\pi\lambda_0^4}\ln\frac{\lambda_H}{\xi} + \delta n_0^2 K_2 \pi \frac{R}{\lambda_H} \\ &+ \delta n_0 K_2 \frac{\lambda_H am}{\lambda_0^2}, \end{aligned} \tag{9}$$

where $m^2 E_{\text{core}}$ is the energy per unit length of destroying the smectic order at the defect core. Note that the strain energy depends not only on the boundary value of $\delta\mathbf{n} = \delta n_0 \phi$, but also on the strength of the defect $m$. When minimizing, we must minimize over *both* variables. Choosing the minimum over $m$ will indicate whether or not there is a screw dislocation at all.

Adding this energy to the surface energy (4), we minimise over $\delta n_0$ to find the minimum energy $\mathcal{F}$. To determine the relative magnitudes of the terms, we estimate $K_2 \approx K_{24} = \mathcal{O}(k_B T/\xi)$ and $a \approx \xi$. In NMR studies [10] it has been seen that $W/K_{24} \approx (28\,\text{nm})^{-1}$ for non-chiral nematic liquid crystal in small capillaries in Nuclepore; we therefore expect that $K_{24}/R \ll W$ for radii in the range of $R \sim 10\,\mu\text{m}$. Thus we find a tipping of

$$\delta n_0 \approx \frac{K_2 q_0}{W}\frac{1 - \dfrac{\lambda_H m a}{2\pi\lambda_0^2 q_0 R}}{1 + \dfrac{K_2}{W\lambda_H}}. \tag{10}$$

For large $R$ the tipping angle at the capillary wall is *independent* of $R$ and $m$. This is because the director can lower the chiral energy by tipping at the wall even in the absence of a defect; the director will align with the layer normal at a distance of a penetration depth from the wall. Therefore we must subtract the strain energy of the zero defect state to arrive at the dislocation energy

$$\begin{aligned} \mathcal{F}/L \approx m^2 &\left\{ E_{\text{core}} + \chi H^2 \frac{a^2\lambda_H^2}{4\pi\lambda_0^2}\ln\frac{R}{\xi} + K_2 \frac{a^2\lambda_H^2}{4\pi\lambda_0^4}\ln\frac{\lambda_H}{\xi} \right\} \\ &+ m\frac{K_2^2 a q_0 \lambda_H}{\left(W + \dfrac{K_2}{\lambda_H}\right)\lambda_0^2}. \end{aligned} \tag{11}$$

We have kept the subleading term $K_2/(W\lambda_H)$ so that our expressions have sensible large $H$ behaviour, for example $\delta n_0 \to 0$, as $H \to \infty$, even though in this limit we leave the type II regime. Each term of (11) has a simple interpretation: the first three terms are the energy of a screw dislocation in a bulk sample subject to a magnetic field, and the last term is the usual chiral term of a bulk defect reduced by a factor involving the anchoring.

Note that if $q_0 = 0$ then the minimum energy is at $m = 0$, in other words, *no defect*. It is easy to see that there are critical values of $H^2$, $R$ and $q_0$ for which the free energy will be minimized for $m \neq 0$. First, we consider zero magnetic field. The sign of the Burgers vector is determined by the sign of $q_0$; we assume that $q_0 > 0$. The critical value of the chirality needed to get a defect with $m = -1$ in a very large capillary ($R \to \infty$) is increased from its bulk value by the anchoring:

$$q_{0c} \approx q_{0c,\text{bulk}}\left(\frac{W\lambda_0}{K_2} + 1\right), \tag{12}$$

where

$$q_{0c,\text{bulk}} = \frac{m}{a}\left[\frac{E_{\text{core}}}{K_2} + \frac{a^2}{4\pi\lambda_0^2}\log(\lambda_0/\xi)\right]. \tag{13}$$

In general the critical chirality depends on the radius. Equivalently, there is a critical radius $R_c$ depending on $q_0$ such that if $R < R_c$, no defect will occur. Unless $q_0$ is very close to its critical value, this radius is typically the size of the penetration depth, in which case our expressions are not valid. We can, of course, compute $R_c$ and its dependence on $W$ by dropping the assumption $R \gg \lambda_0$,

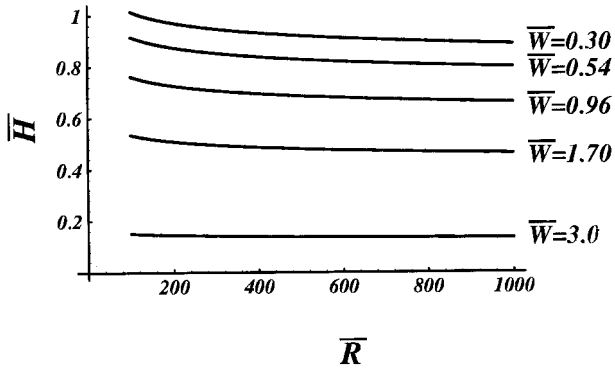


Figure 2. Reduced critical field $\bar{H}$ versus reduced capillary radius $\bar{R}$ for $\bar{W} = 0{\cdot}30$, $0{\cdot}54$, $0{\cdot}96$, $1{\cdot}7$ and $3{\cdot}0$.

but as noted above $R_c$ is not so easy to determine experimentally.

Now consider subjecting the sample to a magnetic field. For a capillary with radius $R > R_c$, there is a critical value $H_c(R, W)$ of the field above which there will be no defect; $H_c(R, W)$ is the number such that the right hand side of (11) is zero for $m \neq 0$. While an analytic expression for $H = H_c$ is complicated, we can easily plot $H_c(R, W)$ for a system in which the elastic constants are known. Thus a given liquid crystal system may be studied in only a few capillaries in order to determine which value of $W$ fits the observed formation of a defect. In fact, due to the logarithmic dependence of the magnetic strain energy on the radius, the critical field is a very weak function of $R$ so that just one measurement may suffice to determine $W$. In figure 2 we show $H_c$ versus $R$ for various $W$, with $R$ ranging over typical capillary sizes of 10–100 μm; $\bar{R} \equiv R/\lambda_0$, $\bar{H}^2 = \chi H^2/B$, $\bar{W} \equiv W \lambda_0/K_2$, and $q_0 = 11\,\mu\text{m}^{-1}$. $\bar{W}$ ranges from 0·3 to 3·0. We have taken $\lambda_0 = 0{\cdot}1\,\mu$m, $4\pi\lambda_0^2 E_{\text{core}}/(a^2 K_2) = 1$, and $\lambda_0/\xi = 10$. Note that the magnetic fields in the ranges we consider do not spoil the type II behaviour since $\lambda_H > \xi$.

## 3. Summary

In summary we have proposed a set of experiments that could be performed on liquid crystals that form TGB phases, such as 3-fluoro-4(1-methylheptyloxy)4′-(4″-alkoxy-2″,3″-difluorobenzyloyloxy)tolane ($nF_2BTFO_1M_7$) [11] which could, in principle, measure the anchoring strength of the capillary wall. Throughout we have neglected the dynamics of the formation of screw dislocations from an undefected sample. The nucleation problem could be avoided experimentally through annealing. It would be an interesting extension of this work, however, to understamnd defect formation. This task would be considerably easier and tremendously more reliable with some experimental input.

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