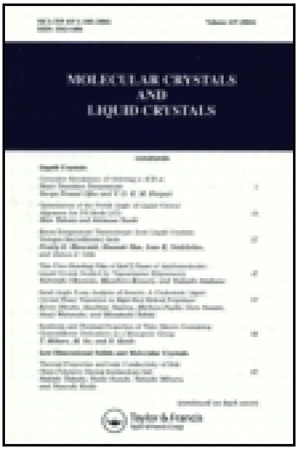

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

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Version of record first published: 05 Oct 2009

Mol. Cryst. Liq. Cryst., Vol. 508, pp. 337/[699]–347/[709], 2009

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400903065853

On the Effect of a Rotating Magnetic Field or Sample on the Bend Freedericksz Critical Field in Nematic Slabs

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A numerical study of the effect of a continuously rotating field or sample on the magnetic Freedericksz transition in homeotropic nematics slabs is presented. Homeotropic boundary conditions with strong anchoring are considered. The magnetic field is applied parallel to the plates, i.e., in the bend Freedericksz geometry. The behaviour of a low molecular weight liquid crystal (5CB) and of a high molecular weight polymer liquid crystal (PBLG) is compared using the Leslie-Ericksen theory of nematodynamics. The effect of the sample thickness, of the magnetic field strength and of the spinning frequency on the response of both materials is studied. Our results show that, in both cases and for both materials, the value of the Freedericksz critical field $H_c(\nu)$ *increases with the spinning frequency* ν*. The transition* $H_c(\nu) \to H_c(0)$ *is found to be continuous in the rotating sample case and to be discontinuous in the rotating field case. The plot of the reduced critical field vs. the reduced spinning frequency gives universal curves for both materials in both cases.*

Keywords: Freedericksz transition; nematic liquid crystal; rotating field; rotating sample

This work was supported in part by FCT of Portugal under Research Contract POCI/CTM/61293/2004.

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INTRODUCTION

The effect in nematic liquid crystals of a continuously rotating sample with a constant magnetic field applied in the plane of rotation or of a rotating field with a stationary sample has been studied since the pioneering work of Gasparoux, Brochard and co-workers [1,2]. It is well known that for a large enough sample in the direction normal to the field or for a strong enough magnetic field, i.e., a field greater than the Freedericksz critical field, the director in the bulk of the sample tends to stay in the plane of rotation [3]. The dynamics of the component of the director in the plane of rotation is reasonably understood, in both cases, when its dependence on the sample thickness is neglected. In the case of the rotating sample, at a critical spinning frequency a transition occurs from a synchronous regime, where the in-plane director keeps with the magnetic field a constant phase lag, to an asynchronous regime, where the phase lag increases with time [1]. A similar behavior occurs in the case of the rotating field, where in the synchronous regime the in-plane director follows the rotating field with constant phase lag, and in the asynchronous regime the phase lag increases with time [2]. A number of complex phenomena may arise during the dynamics in both regimes, such as defect and pattern formation [4–9]. In this work interest is in the comparative numerical study with two very different molecular weight compounds of the change in the Freedericksz threshold as a function of the spinning frequency in both the rotating field and the rotating sample cases, taking in account the dependence of the component of the director in the plane of rotation on the sample thickness and disregarding the problem of the complex dynamics in the plane.

A numerical simulation study of the effect of a rotating field or of a rotating sample on the director field in nematic slabs under an applied magnetic field is thus presented. A nematic monodomain with homeotropic boundary conditions and strong anchoring is considered. The magnetic field is applied normal to the initial director, i.e., in the bend Fredericksz geometry. In this study the response of a low molecular weight liquid crystal (5CB) and of a high molecular weight polymer liquid crystal (PBLG) are compared, using the Leslie-Ericksen theory of nematodynamics [3]. Viscoelastic parameters of both these materials known from the literature are used in the simulations [10,11]. In this analysis a three-dimensional description of the director is used and backflow is neglected. The effect of the sample thickness, of the magnetic field strength and of the rotation frequency on the response of both materials is studied. We focus our study in a spinning frequency range lower than the critical frequency to avoid the asynchronous regime, where backflow coupling should play an important role [7,9].

MATHEMATICAL MODELS

1) Rotating sample

The director and magnetic fields are defined by (see the Figure 1a):

$$
\begin{aligned}
n_x &= \sin(\theta)\cos(\phi) \qquad & H_x &= H \\
n_y &= \sin(\theta)\sin(\phi) \qquad & H_y &= 0 \\
n_z &= \cos(\theta) \qquad & H_z &= 0
\end{aligned}
\tag{1}
$$

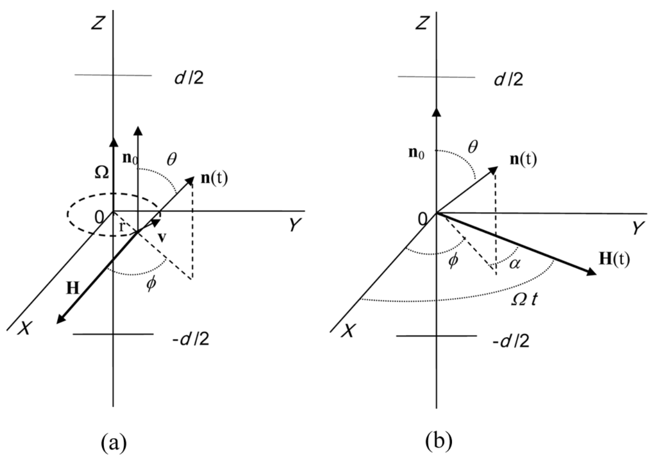

FIGURE 1 Definition of the geometry of the samples. The plates are at $z = \pm d/2$. $\mathbf{n}_0$ is the initial uniform director field, perpendicular to the plates, and $\mathbf{n}(t)$ the director in the central plane of the sample at a given instant. Homeotropic strong anchoring is assumed. A uniform magnetic field $\mathbf{H}$ is applied normal to the initial director. (a) Rotating sample: the reference frame XYZ rotates with angular velocity Ω and the magnetic field is constant and set in the OX direction; the local director is at a point located at a distance *r* from the origin; (b) Rotating field: the reference frame XYZ is fixed and the magnetic field rotates in the XY plane with constant angular velocity Ω; the local director is at the origin for convenience.

The velocity field is assumed to be the linear velocity of a rigid cylinder of angular velocity Ω. This approximation will allow uncoupling the director from the velocity in the dynamic equations [8].

$$\begin{aligned} v_x(y) &= -\Omega y \\ v_y(x) &= \Omega x \\ v_z &= 0 \end{aligned} \tag{2}$$

These functions obey the incompressibility condition. The homeotropic rigid boundary conditions of the director will be approximated taking only in account the first harmonic term in a Fourier expansion of the director field, which is the leading term:

$$\begin{aligned} \theta(z,t) &= \theta_0(t)\cos(q_z z) \\ \phi(z,t) &= \phi_0(t)\cos(q_z z) \end{aligned} \tag{3}$$

Here q_z is the wavevector of the distortion in the OZ direction, where d is the sample thickness:

$$q_z \approx \frac{\pi}{d} \tag{4}$$

Next the functions (1) to (4) are plugged in the Ericksen-Leslie equations [3]. A non dimensional time variable is chosen:

$$t' = \frac{t}{\tau_0}; \quad \tau_0 = \frac{2\gamma_1}{\chi_a H^2} \tag{5}$$

Here $\gamma_1 = \alpha_3 - \alpha_2$ is the rotational viscosity, where α_2 and α_3 are Leslie viscosity coefficients and χ_a is the anisotropy of the magnetic susceptibility. After some algebra, the following two independent non dimensional equations result for the time evolution of the angles $\theta_0(t')$ and $\phi_0(t')$ in the central plane of the sample ($z = 0$), after dropping the subscript 0 and the explicit time dependence for simplicity:

$$\frac{d\theta}{dt'} = \cos^2(\phi)\sin(2\theta) + \delta\frac{f_1(\theta)}{K_3}\theta \tag{6}$$

$$\frac{d\phi}{dt'} = \nu - \sin(2\phi) + \delta\frac{f_2(\theta)}{K_3}\phi \tag{7}$$

In these equations, the functions

$$f_1(\theta) = -K_1 - K_3 + (K_1 - K_3)\cos(2\theta) \tag{8}$$

$$f_2(\theta) = -K_2 - K_3 + (K_2 - K_3)\cos(2\theta) \tag{9}$$

are elastic terms, where K_1, K_2 e K_3 are the splay, twist and bend Frank constants, and two non dimensional numbers show up, which are the control parameters in our simulations:

1) The ratio of the (density of) elastic energy and the (density of) magnetic energy:

$$\delta = \frac{K_3 q_z^2}{\chi_a H^2} = \frac{H_c^2}{H^2} = \frac{1}{h^2} \tag{10}$$

where H_c is the Freedericksz critical field [3] and h is the reduced field.

2) The ratio of the spinning frequency Ω and the critical frequency Ω_c:

$$\nu = \frac{\Omega}{\Omega_c}; \quad \Omega_c = \frac{1}{\tau_0} \tag{11}$$

The critical frequency defines the transition from the synchronous state ($\Omega < \Omega_c$), where the component of the director in the plane of rotation follows the rotating field with constant phase lag $\phi < \pi/4$, to the asynchronous regime ($\Omega > \Omega_c$), where ϕ increases monotonously with time, when its dependence on the sample thickness is neglected [1]. This critical frequency can be easily obtained from equation (7) with (11) in the limit $d \to \infty$, i.e when the elastic torques arising from the boundaries on the component of the director in the plane of rotation are neglected at the central plane of the sample, and solving for the stationary solution of the phase lag:

$$\phi = \frac{1}{2} arc\sin(\nu), \quad \text{when} \quad \nu \leq \nu_c = 1 \tag{12}$$

2) Rotating field

The director and magnetic fields are defined by (see the Figure 1b):

$$\begin{aligned} n_x &= \sin(\theta)\cos(\phi) & H_x &= H\cos(\Omega t) \\ n_y &= \sin(\theta)\sin(\phi) & H_y &= H\sin(\Omega t) \\ n_z &= \cos(\theta) & H_z &= 0 \end{aligned} \tag{13}$$

Under the same harmonic approximation as in the previous section, the velocity and the director fields are taken respectively as:

$$\begin{aligned} v_x(z,t) &= v_{0x}(t)\cos(q_z z) \\ v_y(z,t) &= v_{0y}(t)\cos(q_z z) \\ v_z &= 0 \end{aligned} \tag{14}$$

$$\begin{aligned} \theta(z,t) &= \theta_0(t)\cos(q_z z) \\ \phi(z,t) &= \phi_0(t)\cos(q_z z) \end{aligned} \tag{15}$$

where q_z is the wavevector of the distortion in the OZ direction, given by (5).

Proceeding as in the previous section, the functions (1) to (4) are plugged in the Ericksen-Leslie equations, the non dimensional time variable (5) is chosen and the following equations in the central plane of the sample are obtained:

$$\frac{d\theta}{dt'} = \cos^2(\nu t' - \phi)\sin(2\theta) + \delta\frac{f_1(\theta)}{K_3}\theta \tag{16}$$

$$\frac{d\phi}{dt'} = \sin[2(\nu t' - \phi)] + \delta\frac{f_2(\theta)}{K_3}\phi \tag{17}$$

As a consequence of our approximations, in these equations the director field gets uncoupled from the velocity field, as in the previous problem. The elastic functions $f_1(\theta)$ and $f_2(\theta)$ are also defined by (8) and (9) respectively and the control parameters are again δ given by (10) and ν given by (11). In this problem the critical frequency also defines the transition from the synchronous to the asynchronous regime of component of the director in the plane of rotation, when its dependence on the sample thickness is neglected [2]. When no elastic torques arising from the boundaries act at the central plane of the sample, this critical frequency can be easily obtained from equation (17) with (5), in the limit d $\to \infty$ and solving for the stationary solution of the phase lag $\alpha = \Omega t - \phi$:

$$\alpha = \frac{1}{2} arc\sin(\nu), \quad \text{when } \nu \leq \nu_c = 1 \tag{18}$$

RESULTS

1) Rotating sample

The system of equations (6) and (7) is solved numerically with the parameters of 5CB or PBLG of Table 1, for given values of the control parameters δ and ν defined by (10) and (11). We focus our study in the non dimensional spinning frequency range $0 \leq \nu < 1$ to avoid the more complex asynchronous regime, where backflow coupling plays an important role [7,9]. We also study the range $0 \leq \delta \leq 1$, where the lower limit corresponds to an infinite value of the reduced field, i.e., infinite

TABLE 1 Parameters used in the numerical simulations

5CB[10]	PBLG[11]
$\alpha_2 = -0.77\,\mathrm{g\,cm^{-1}\,s^{-1}}$	$\alpha_2 = -1.328\times10^4\,\mathrm{g\,cm^{-1}\,s^{-1}}$
$\alpha_3 = -0.042\,\mathrm{g\,cm^{-1}\,s^{-1}}$	$\alpha_3 = 40.00\,\mathrm{g\,cm^{-1}\,s^{-1}}$
$K_1 = 5.95\times10^{-7}$ dyn	$K_1/K_2 = 52.4$
$K_2 = 3.77\times10^{-7}$ dyn	$K_3/K_2 = 30.1$
$K_3 = 7.86\times10^{-7}$ dyn	$K_2 = 0.6\times10^{-7}$ dyn

The materials under consideration are the nematic phase of 5CB (4-pentyl-4′-cyanobiphenyl) [10] and of PBLG (poly-γ-benzyl-L-glutamate) in m-cresol (17 wt% PBLG/m-cresol, Mn = 280 000, $T = 302$ K [12]).

applied magnetic field or sample dimension in the z direction, and the upper limit corresponds to the Freedericksz threshold when $\nu = 0$. In the Figure 2 is shown the behaviour of the polar angle θ, after discarding transient values, as a function of the parameter δ, for (a) $\nu = 0$ and b) $\nu = 0.2$. Even though two different curves show up for 5CB (1) and PBLG (2), the limit values are the same for both materials with the same values of the control parameters. When $\nu = 0$ we find that θ goes from $\pi/2$ for $\delta = 0$ to zero for $\delta = 1$. The first limit corresponds to a director that lies in the plane of rotation, while the second limit corresponds to the usual Freedericksz transition, as expected. For $\nu > 0$ this critical value of δ gets smaller, as shown in the Figure 2b for the particular case $\nu = 0.8$ and in the Figure 3 as a function of ν, where the same curve shows up for both materials. This means that

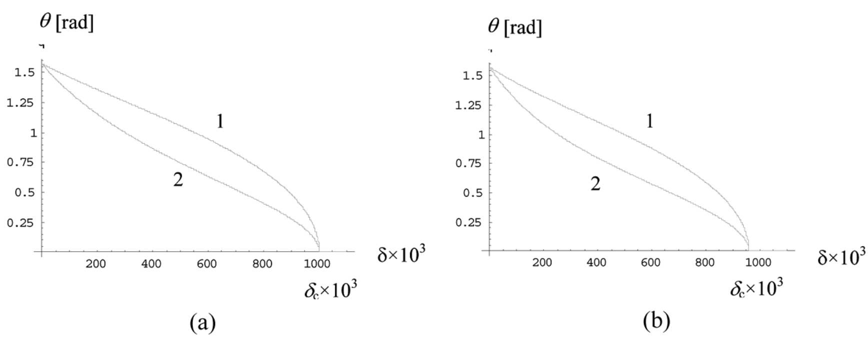

FIGURE 2 Rotating sample. Plot of the stationary value of the polar angle θ, from the solution of the system (6,7) for late times, as a function of the parameter δ, computed with the parameters of 5CB (1) and PBLG (2) for (a) $\nu = 0$; (b) $\nu = 0.8$.

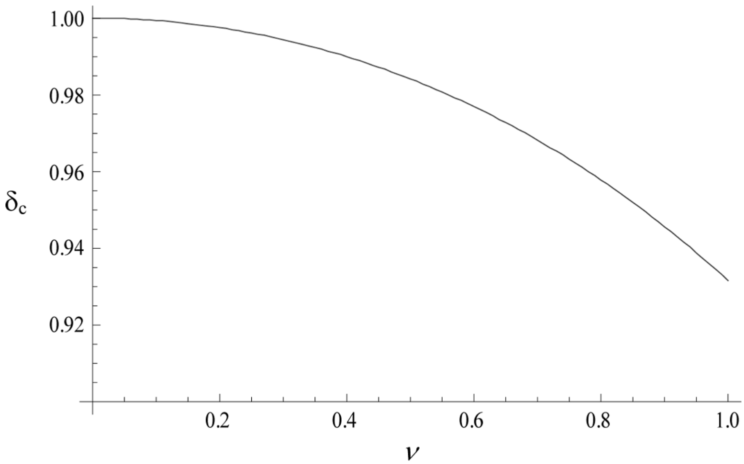

FIGURE 3 Rotating sample. Critical value of δ as a function of ν. Same curve for 5CB and PBLG.

the critical reduced field increases with the spinning frequency. The transition to $\delta = 1$ at $\nu = 0$ is found to be continuous.

2) Rotating field

The same method is followed as in 1). The results are shown in the Figures 4 and 5 and are similar to those found in the rotating field case, except that the transition at $\nu = 0$ is found to be discontinuous in this case.

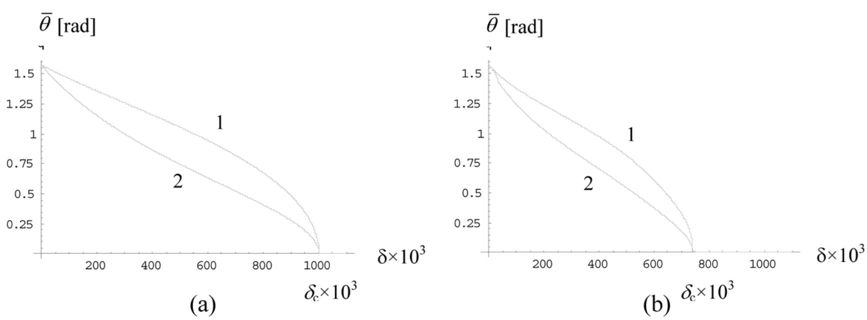

FIGURE 4 Rotating field. Plot of the average value of the polar angle, from the solution of the system (16,17) for late times, as a function of the parameter δ, computed with the parameters of 5CB (1) and PBLG (2) for (a) $\nu = 0$; (b) $\nu = 0.2$.

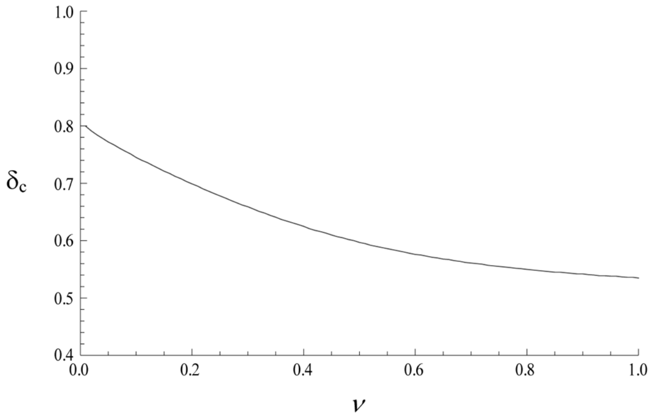

FIGURE 5 Rotating field. Critical value of δ as a function of ν. Same curve for 5CB and PBLG.

DISCUSSION

The increasing of the critical field with the spinning frequency can be explained in terms of an effective field acting on the nematic director, $H\cos(\phi)$ in the rotating sample case and $H\cos(\alpha)$ in the case of the rotating field [2]. In the first case, from a stability analysis of equations (6,7), when $\theta = 0$, there results a frequency dependent effective critical field

$$H_c(\nu) = \frac{H_c(0)}{\cos(\phi)} \tag{19}$$

Together with the result (12) this effective critical field can be written in terms of the dimensionless frequency ν

$$\frac{H_c^2(\nu)}{H_c^2(0)} = \frac{2}{1+\sqrt{1-\nu^2}} \tag{20}$$

From this result two interesting limits can be obtained:

$$\begin{aligned} \lim_{\nu\to 0} H_c(\nu) &= H_c(0) \\ \lim_{\nu\to 1} H_c(\nu) &= \sqrt{2}H_c(0) \end{aligned} \tag{21}$$

The first limit gives the threshold field for the distortion in the static regime and the second limit gives the threshold in the asynchronous regime, as found in [2] for the rotating field case when neglecting the influence of the boundaries on the in-plane director component. From this analysis the transition at $\nu = 0$ to the static critical field value is predicted by equation (20) to be continuous in the rotating sample case, in agreement with the curve shown in the Figure 3.

In the rotating field case, the critical field obtained via our non linear analysis and plotted in the Figure 5 does not follow a continuous path to $\delta = 1$ when $\nu \to 0$. It can be shown theoretically that, in this limit, the critical field jumps discontinuously from 0.8 to 1 [13]. This will be discussed elsewhere together with the theoretical proof that, in both cases studied here, the curves $\delta_c(\nu)$ in the Figures 3 and 5 are universal curves, i.e., independent of the material parameters, as suggested by the numerical results presented here.

CONCLUSIONS

Our results show that, in both the rotating sample and the rotating field problems and for both low molecular and polymer materials, the value of the effective Freedericksz critical field $H_c(\nu)$ increases with the spinning frequency ν. The transition $H_c(\nu) \to H_c(0)$ is found to be continuous in the rotating sample case, while it is discontinuous in the rotating field case. In spite of the anisotropy of the viscoelastic parameters differ appreciably from one material to the other, the plot of the reduced critical field vs. the reduced rotation frequency in each problem gives the same curves for both materials, i.e., universal curves.

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