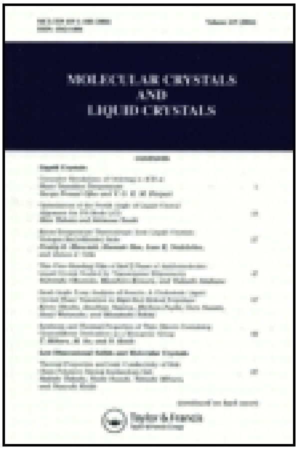

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Analysis of the Shear-Induced Pattern Formation in Nematic Polymer Liquid Crystals Under an Applied Magnetic Field

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The formation of the shear induced periodic patterns in the nematic polymer liquid crystal PBG is studied using linear stability analysis of the Leslie–Ericksen equations for shear flow. The unidirectional shear of a nematic director initially uniformly oriented orthogonally to the sample plane and with strong anchoring is considered. The stabilizing effect of a magnetic field applied in the same direction is studied. The results show that for tumbling nematics critical values of the Ericksen number and of the applied magnetic field show up for which the uniform flow may become unstable to a periodic tilting of the director out of the shearing plane, giving rise to a periodic band structure orthogonal to the shearing.

Keywords: nematic; pattern; polymer; shear

1. INTRODUCTION

The analysis of the shear and the field induced instabilities is a significant subject in the polymer liquid crystal (PLC) science [1–5]. In slow enough flows so that the equilibrium shape of the macromolecules remains unaltered in spite of flow, the behaviour of polymeric nematics is well described by the Leslie–Ericksen theory [2,3]. In this work, the formation of the shear induced periodic patterns in the nematic polymer liquid crystal PBG is studied using linear stability analysis of the Leslie–Ericksen equations [6] for shear flow. Such an

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analysis should give a sufficiently good understanding of the processes at work, if not a quantitative account [7]. The unidirectional shear of a nematic director initially uniformly oriented orthogonally to the sample plane and with strong anchoring is considered. The stabilizing effect of a magnetic field applied in the same direction is studied. After the start-up of shearing the director rotates towards the shear direction. The results show that for tumbling nematics a periodic instability may show up. Depending on the values of the control parameters, at an angle θ_c with respect to the initial homeotropic alignment of the director the uniform flow may become unstable to a periodic tilting of the director out of the shearing plane, giving rise to a periodic band structure orthogonal to the shearing, as observed experimentally [8]. This result was obtained for two different sets of viscoelastic parameters of solutions of PBG (see the Table 1), corresponding to samples of different molecular weight. For both these samples the ratio of Leslie viscosities α_2/α_3 is negative, corresponding to the tumbling nematic type. For the parameters of the flow aligning low molecular weight nematics 5CB [14] and MBBA [6], the calculation shows that the uniform flow is stable against periodic perturbations. These results are consistent with the known fact that tumbling nematics are susceptible to instabilities that drive the director towards the vorticity direction [1,9]. The critical director orientation angle with respect to the shear direction for the selection of a periodic pattern is analogous of the critical angle with respect to the magnetic field in the field induced patterns [10,11]. For not too great values of the Ericksen number and/or not too weak applied magnetic fields the flow is such that the director gets aligned in the shearing plane at a limiting angle $\theta_m > \theta_c$. The stability analysis of this stationary solution of the dynamic equations gives qualitatively similar results as for θ_c

TABLE 1 Parameters Used in the Numerical Simulations

PBG 1 [5]	PBG 2 Viscosities [2] Elastic constants [13]
$\alpha_1 = -36.7\,(\mathrm{g\,cm^{-1}\,s^{-1}})$	$\alpha_1 = -1.212 \times 10^4\,(\mathrm{g\,cm^{-1}\,s^{-1}})$
$\alpha_2 = -69.2$	$\alpha_2 = -1.328 \times 10^4$
$\alpha_3 = 0.20$	$\alpha_3 = 40.00$
$\alpha_4 = 3.48$	$\alpha_4 = 1.137 \times 10^3$
$\alpha_5 = 66.1$	$\alpha_5 = 1.208 \times 10^4$
$K_1 = 12.1\,(10^{-7}\mathrm{dyn})$	$K_1/K_2 = 52.4$
$K_2 = 0.78$	$K_3/K_2 = 30.1$
$K_3 = 7.63$	$K_2 = 0.6 \times 10^{-7}\,(\mathrm{dyn})$

although producing different critical values of the control parameters for the onset of the periodic instability.

2. MATHEMATICAL MODEL

An aligned nematic monodomain between two parallel plates with homeotropic boundary conditions and rigid anchoring and with positive anisotropy of the magnetic susceptibility χ_a is considered. An unidirectional shear with constant velocity V is applied to the plates in opposite directions parallel to their plane and an uniform magnetic field is applied normally to the sample plane as shown in Figure 1.

In order to study the stability of the uniform flow with respect to periodic perturbations out of the shearing plane that result in bands orthogonal to the shear direction, the following magnetic, velocity

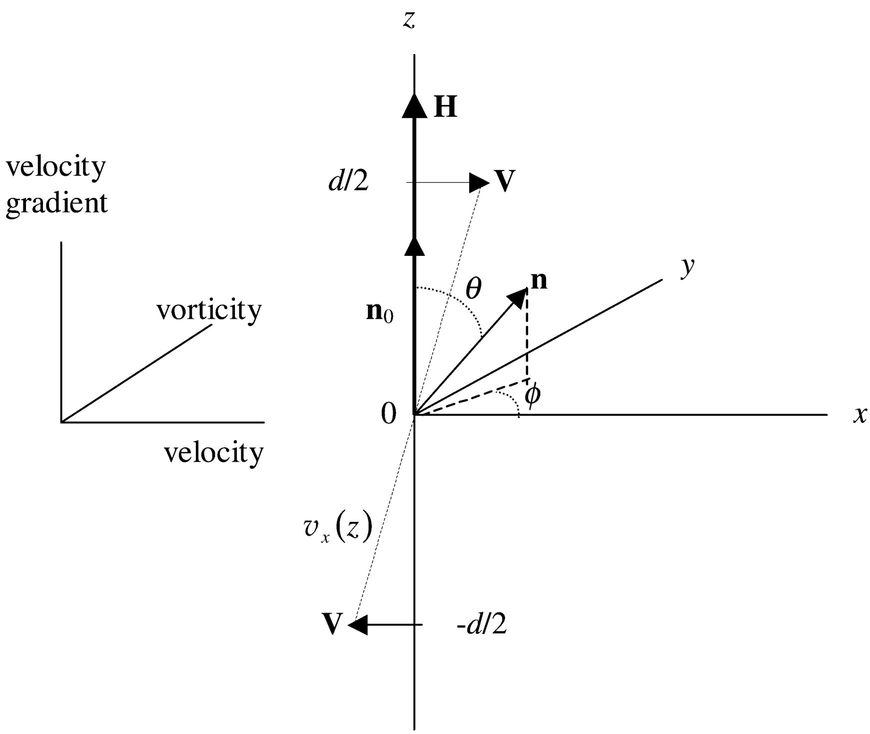

FIGURE 1 Definition of the sample geometry. The plates are at $z = \pm d/2$. $\mathbf{n}_0$ is the initial uniform director field and $\mathbf{n}$ its direction at a given instant during the flow.

and director fields are taken

$$\begin{aligned} &H_x = 0,\ H_y = 0,\ H_z = H \\ &v_x(z),\ v_y(x,z,t),\ v_z = 0 \\ &n_x = \sin\theta(z,t)\cos\ \phi(x,z,t), \\ &n_y = \sin\ \theta(z,t)\sin\ \phi(x,z,t), \\ &n_z = \cos\ \theta(z,t) \end{aligned} \tag{1}$$

Following the perturbation method described in [10] the following functions for the velocity and the director fields are considered:

$$\begin{aligned} v_x(z) &= \dot{\gamma} z \\ v_y(x,z,t) &= 0 + \xi_v(x,z,t) \\ \theta(z,t) &= \theta_0(t) f(z) \\ \phi(x,z,t) &= 0 + \xi_\phi(x,z,t) \end{aligned} \tag{2}$$

In the rhs of (2) the first terms correspond to the uniform flow, where $\dot{\gamma}$ is the shear rate, and the second terms in v_y and ϕ are the perturbations of the velocity and the director fields respectively. Following [7] the single mode approximation in both the x and the z directions will be used in (2):

$$\begin{aligned} f(z) &= \cos(q_z z) \\ \xi_v(x,z,t) &= v_0(t)\sin(q_x x)\cos(q_z z) \\ \xi_\phi(x,z,t) &= \phi_0(t)\cos(q_x x)\cos(q_z z) \end{aligned} \tag{3}$$

Approximate boundary conditions are set through the condition

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

where q_x and q_z are the cartesian components of the wavevector of the distortion and d is the sample thickness in the OZ direction. The functions (3) with (4) represent harmonic distortions that obey the boundary conditions at $z = \pm d/2$, corresponding to the no slip condition for the velocity and to homeotropic alignment for the director.

Inserting the fields (1–4) in the the Leslie–Ericksen equations one gets in the central plane of the sample ($z = 0$) the following variational equations up to the first order in the perturbations ξ_v and ξ_ϕ, where the functions $\theta_0(t)$, $v_0(t)$ and $\phi_0(t)$ will be shortened to θ, v and ϕ for simplicity

$$\gamma_1 \frac{d\phi}{dt} = \left\{\alpha_2 \dot{\gamma}\cot\theta - \left[q_z^2 f(\theta) + q_x^2 g(\theta)\right]\right\}\phi - \alpha_2 q_x v \equiv \gamma_1 F_\phi \tag{5}$$

$$\rho \frac{dv}{dt} = -\alpha_2 q_x \sin^2\theta \frac{d\phi}{dt} + q_x \frac{1}{2}\sin(2\theta)\left[\mu(\theta)\dot{\gamma} - \gamma_2 \frac{d\theta}{dt}\right]\phi \\ - \left[q_z^2 \gamma(\theta) + q_x^2 \eta(\theta)\right] v \tag{6}$$

where

$$f(\theta) = K_2 \sin^2\theta + K_3 \cos^2\theta \tag{7}$$

$$g(\theta) = K_2 \cos^2\theta + K_3 \sin^2\theta \tag{8}$$

$$\mu(\theta) = \frac{1}{2}\alpha_3 - \frac{1}{2}\alpha_6 - \alpha_2 - \alpha_1 \sin^2\theta \tag{9}$$

$$\gamma(\theta) = \eta_c \cos^2\theta + \eta_a \sin^2\theta \tag{10}$$

$$\eta(\theta) = \eta_c \sin^2\theta + \eta_a \cos^2\theta \tag{11}$$

and the non-perturbed equation for the flow in the shearing plane:

$$\gamma_1 \frac{d\theta}{dt} = \left(\alpha_3 - \gamma_2 \cos^2\theta\right)\dot{\gamma} - q_z^2 \theta h(\theta) - \frac{1}{2}\chi_a H^2 \sin(2\theta) \tag{12}$$

where

$$h(\theta) = K_1 \sin^2\theta + K_3 \cos^2\theta \tag{13}$$

and where the parameters are the Leslie coefficients α_i, $i = 1, \ldots, 5$, $\alpha_6 = \alpha_3 + \alpha_2 + \alpha_5$, the rotational viscosities $\gamma_1 = \alpha_3 - \alpha_2$ and $\gamma_2 = \alpha_3 + \alpha_2$, the Miesowicz viscosities $2\eta_a = \alpha_4$, $2\eta_b = \alpha_3 + \alpha_4 + \alpha_6$ and $2\eta_c = \alpha_4 + \alpha_5 - \alpha_2$, the Frank elastic constants K_i, i = 1, 2, 3 [6], and the density ρ.

To perform a stability analysis the system of equations (5), (6) and (12) is put in canonical form with the substitution of both $d\theta/dt$ as given by (12) and $d\phi/dt$ as given by (5) in the equation (6), from which there results the following equation:

$$\rho \frac{dv}{dt} = q_x \frac{1}{2}\sin(2\theta)\left\{\begin{array}{c} \nu(\theta)\dot{\gamma} + \dfrac{\alpha_2}{\gamma_1}\tan\theta\left[q_z^2 f(\theta) + q_x^2 g(\theta)\right] \\ + \dfrac{\gamma_2}{\gamma_1} q_z^2 \theta h(\theta) + \dfrac{1}{2}\chi_a H^2 \sin(2\theta) \end{array}\right\}\phi \\ + \left\{q_x^2\left[\frac{\alpha_2^2}{\gamma_1}\sin^2\theta - \eta(\theta)\right] - q_z^2 \gamma(\theta)\right\} v \equiv \rho F_v \tag{14}$$

where

$$\nu(\theta) = \mu(\theta) + \frac{\gamma_2^2}{\gamma_1}\cos^2\theta - \frac{\alpha_2^2}{\gamma_1} - \frac{\alpha_3\gamma_2}{\gamma_1} \tag{15}$$

Although linear in the perturbations, the system of equations (5) and (14) gives a non-linear description of the flow in terms of θ. The local dynamical and structural stability properties of the system at the transition point are determined by the eigenvalues of the stability matrix $F_{ij} \equiv \partial F_i/\partial j$, where $i,\ j = \phi, v$ and the functions F_i are defined in the equations (5) and (14). In the systems under study in this work both eigenvalues turn out to be real and unequal. In this case there is a bifurcation when at least one eigenvalue assumes the value zero. The critical wavevector q_c of the periodic mode is found maximizing the growth rate σ of the instability, which is defined as the eigenvalue that undergoes a change of sign at the transition point. The corresponding critical growth rate is $\sigma_c \equiv \sigma(q_c)$. The behaviour of both the critical growth rate and the critical wavevector as a function of the control parameters will give the necessary information about the stability properties of the nematic system under shear flow.

A scaling analysis is carried out with the following choice of non-dimensional variables:

$$t' = \frac{K_2 q_z^2}{|\alpha_2|}t;\ \ v' = \frac{|\alpha_2|}{K_2 q_z}v \tag{22}$$

from which there results the non-dimensional wavevector

$$q' = \frac{q_x}{q_z} \tag{23}$$

and with q_z given by (4) a rough estimate of the Ericksen number is obtained

$$Er = \frac{|\alpha_2|\dot{\gamma}d^2}{K_2} \tag{24}$$

Two more interesting non-dimensional ratios can be obtained from the scaled equations: the square reduced magnetic field

$$h^2 = \left(\frac{H}{H_c}\right)^2, \quad H_c^2 = \frac{K_2\pi^2}{\chi_a d^2} \tag{25}$$

where H_c is the Freedericksz critical Field [6], and the magnetic to viscous energy ratio

$$\delta = \frac{\chi_{\rm a} H^2}{|\alpha_2|\dot{\gamma}} \tag{26}$$

3. RESULTS

Following the method described at the end of the previous section, the critical wavevector q_c and the critical growth rate σ_c are numerically calculated as a function of θ with the two sets of viscoelastic parameters of PBG given in the Table 1. The numerical results are invariant for constant Er and h or, equivalently, for constant Er and δ. At an angle θ_c with respect to the initial homeotropic alignment of the director the uniform flow may become unstable to a periodic tilting of the director out of the shearing plane, giving rise to a periodic band structure orthogonal to the shearing. In the Figure 2 are shown the critical wavevector and the critical growth rate as a function of θ for the more viscous sample and for $d = 30\,\mu m$, $\dot{\gamma} = 0.1$ and $\chi_a H^2 = 20$. A critical value θ_c shows up above which the periodic instability may develop. For not too great values of the Ericksen number and/or not too weak applied magnetic fields the flow is such that the director gets aligned in the shearing plane at a limiting angle $\theta_m > \theta_c$. In the Figure 2 it can be seen that the overall maximum of the critical growth rate lies away from $\theta_c = 12^\circ$ and twelve degrees before $\theta_m = 88^\circ$. This predicts that although the uniform flow may become unstable for periodic perturbations out of the shearing plane before reaching the stationary solution, a prediction supported by an analysis based on the time dependent solution of the dynamic equations (5), (6) and (12) [12], the bands should appear after a substantial alignment of the director toward the flow, as shown by experiments on high molecular weight samples of PBG in a similar geometry [8]. The wavelength computed at θ_m is $\lambda = 26\,\mu m \cong d$ and in good agreement with the experimental values of [8]. The transition is subcritical (both at θ_c and at θ_m), as can be seen in the Figures 2, 3 and 4. For zero applied magnetic field the values of θ_c and of θ_m are found to depend only on the Ericksen number. A critical value Er_c shows up, *below* which the uniform flow is stable. When a magnetic field is applied normally to the sample plane the value of the critical Ericksen number is found to increase and to diverge at a critical value of the ratio δ, *above* which the uniform flow is stable, as can be seen in the Figure 5 from the analysis at θ_m for the less viscous sample. The stability analysis at θ_c gives results qualitatively similar to the ones found at θ_m, although producing a smaller critical Ericksen number ($Er_c = 694.5$) and a greater critical value of the ratio δ ($\delta_c = 2.3$) for the less viscous sample. Consequently, the instability may develop for values of the Ericksen number smaller and for values of the parameter δ greater than the critical values predicted for the onset of the instability of the

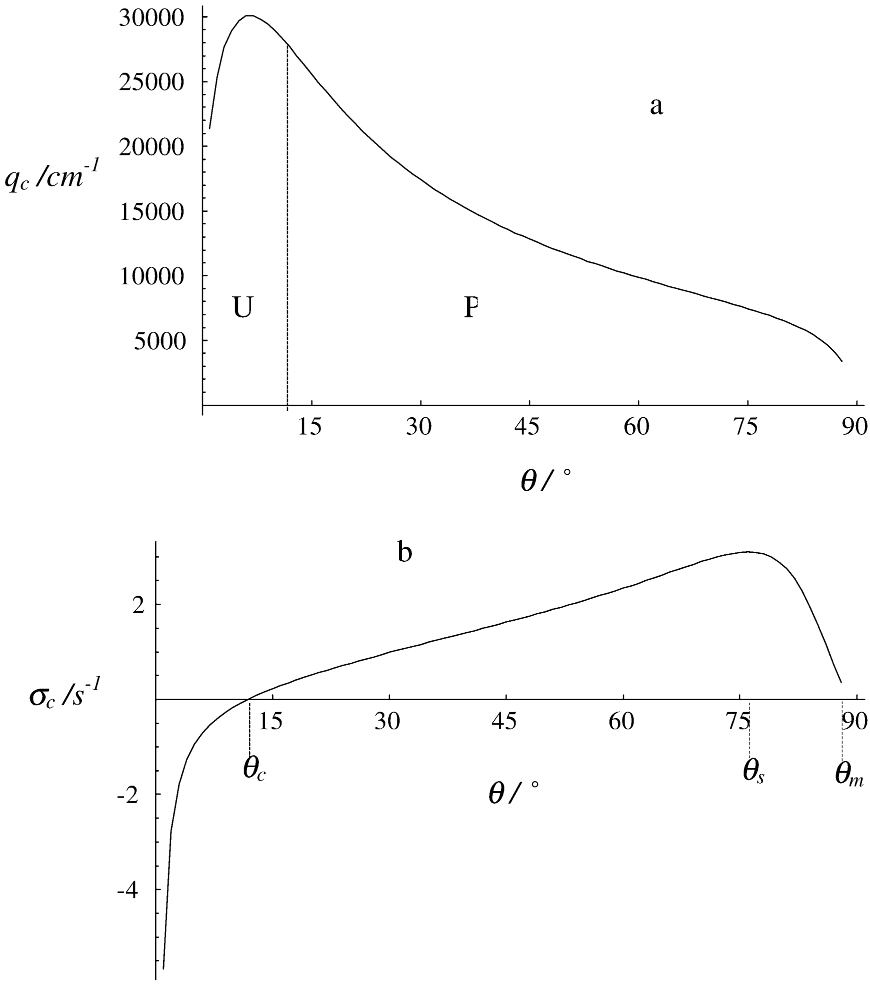

FIGURE 2 Critical wavevector (a) and critical growth rate (b) as a function of θ with the parameters of PBG 2 and with $d = 30\,\mu\text{m}$, $\dot{\gamma} = 0.1$ and $\chi_a H^2 = 20$, from which there results $Er = 199200$ and $\delta = 0.015$, which means that the influence of the magnetic field is almost negligible in this case. The critical angle is $\theta_c = 12^\circ$, the maximum of the critical growth rate is at $\theta_s = 76^\circ$ and the stationary solution is $\theta_m = 88^\circ$. The functions (a) and (b) are not defined at $\theta = 0^\circ$. When θ goes from 0° to θ_m the transition at θ_c is subcritical as can be seen from the curve (a). U = uniform , P = periodic.

stationary solution in this case. For the more viscous sample under ordinary experimental conditions the value of δ_c correspond to unrealistically strong magnetic fields.

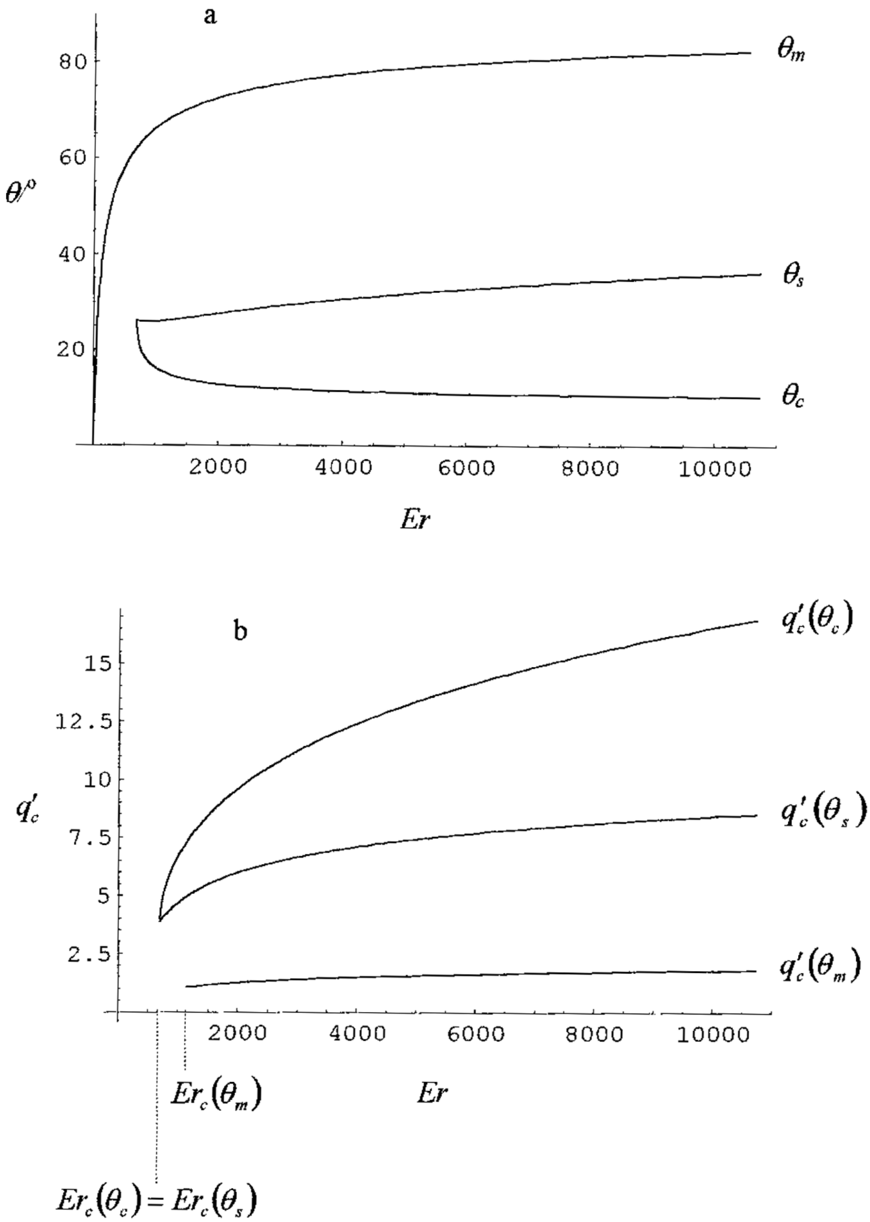

FIGURE 3 (a) angles θ_c, θ_s and θ_m and (b) the corresponding values of the reduced critical wavevector q_c' as a function of *Er* with the parameters of PBG 1. The transitions at $\sigma_c(\theta_c) = 0$, $\sigma_c(\theta_s) = 0$ and $\sigma_c(\theta_m) = 0$ are subcritical and give for the critical Ericksen number respectively the values $Er_c(\theta_c) = Er_c(\theta_s) = 694.5$ and $Er_c(\theta_m) = 1149.8$.

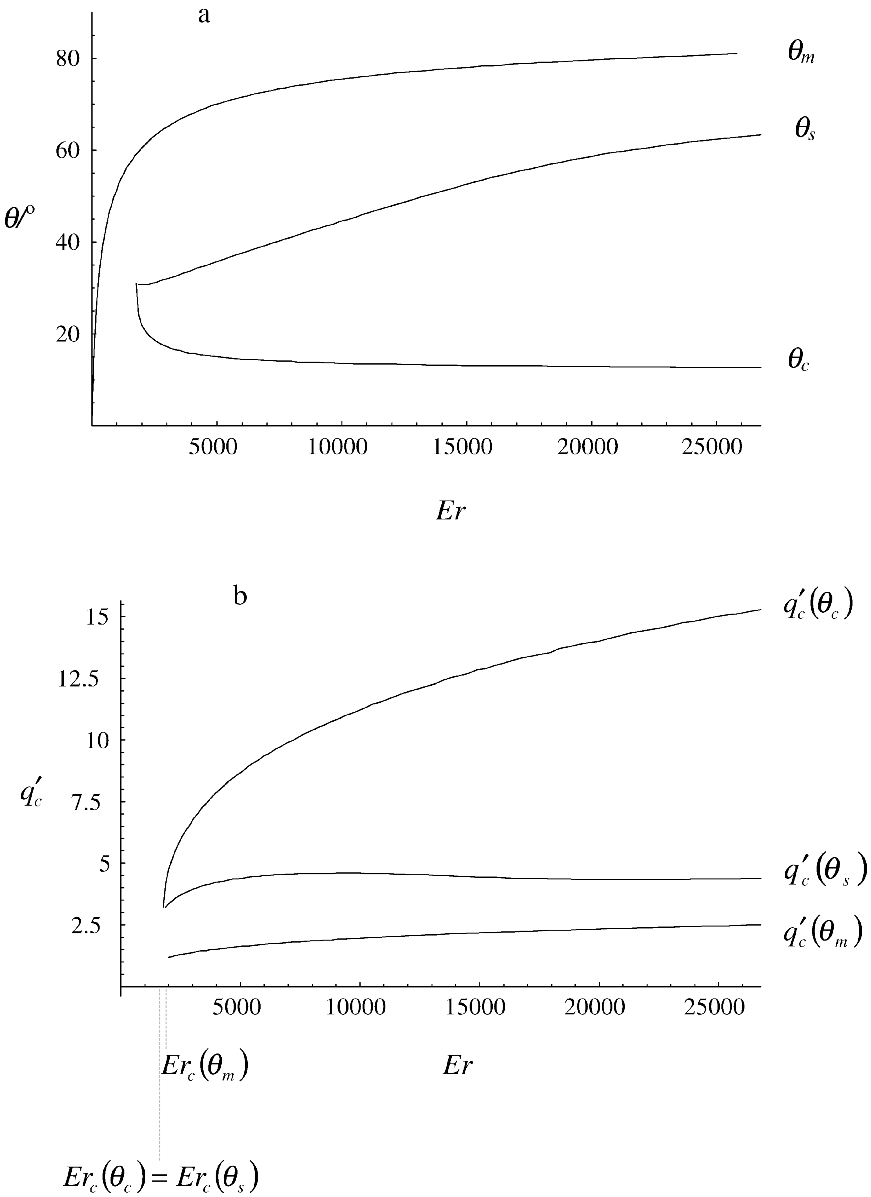

FIGURE 4 The same functions as in the Figure 8 with the parameters of PBG 2; $Er_c(\theta_c) = Er_c(\theta_s) = 1766.6$ and $Er_c(\theta_m) = 1992$.

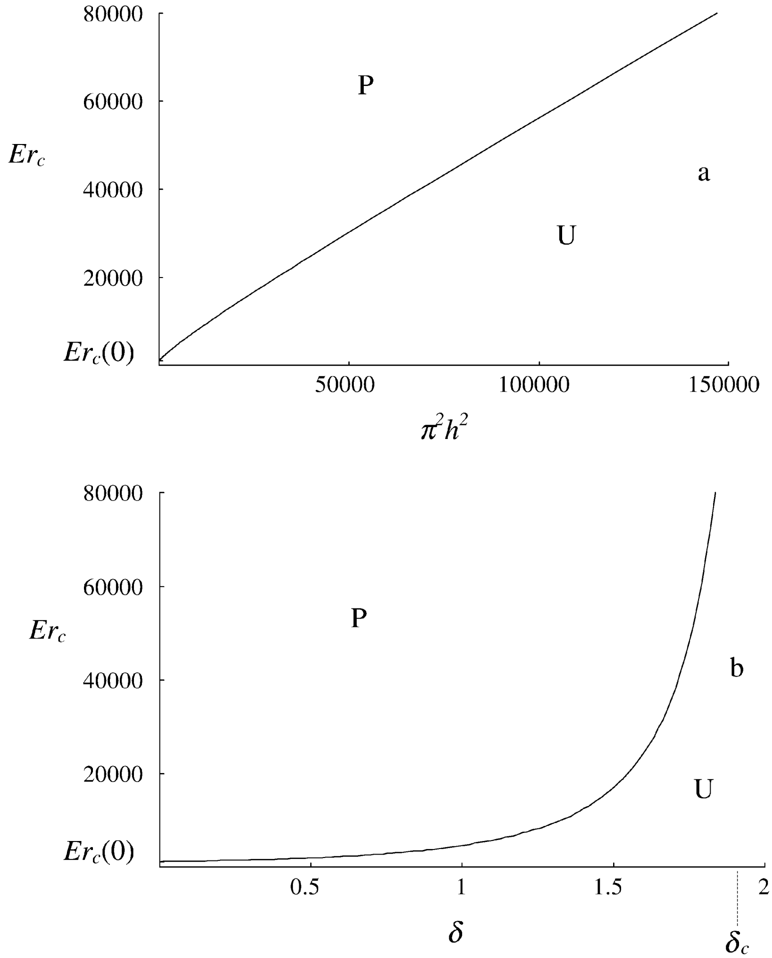

FIGURE 5 Analysis at θ_m of the critical Ericksen number with the parameters of PBG 1 as a function of (a) $\pi^2 h^2$, where h is the reduced field given by (25), and (b) δ given by (26). U = uniform, P = periodic. $\delta_c = 1.9$.

4. CONCLUSIONS

The linear stability analysis of the Leslie–Ericksen equations for shear flow of tumbling nematic polymers with homeotropic boundary conditions and with a magnetic field applied orthogonally to the sample plane predict the possibility of the formation of transient bands orthogonal to the shearing direction, as observed experimentally. Critical values of the Ericksen number of the flow and of the applied magnetic field show up. Consequently, for a given shear rate the formation of the bands may be prevented with a sufficiently thin sample and/or a sufficiently strong magnetic field applied normally to the sample plane in order that the homeotropic alignment of the director is reinforced. Since the transient bands studied in this work are one pathway to the formation of steady-state stripes parallel to the shearing direction [8], the stabilization of the flow may possibly be achieved through the prevention of the formation of the bands as suggested in this work.

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