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Simulation of transient banded textures of sheared nematic polymers

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Nematic polymers, under certain conditions, develop a transient banded texture after cessation of simple shear flow when observing the sheared sample between crossed polars. Here we present a viscoelastic model that describes the formation mechanism of this well-characterized but yet unexplained phenomenon for a typical uniaxial rigid rod nematic polymer. It predicts that the relaxation of shear-flow enhanced scalar order parameter spatial fluctuations produces spatially periodic torques on the director, thereby producing a transient banded texture when viewing the sample between crossed polars. Our numerical results and digitized optical pattern are in good agreement with reported experimental observations.

An intriguing characteristic property of nematic and cholesteric polymers is the formation of a transient banded texture after cessation of shear flow observed when viewing the sample between crossed polars with one of the polars parallel to the prior shearing direction [1–14]. The transient banded texture consists of fine and equally spaced black lines perpendicular to the prior shearing direction, and only forms if the previously applied shear rate and shearing time exceed certain critical values [7–12]. The spatial distribution of the average molecular orientation, defined by a unit vector called the director $\mathbf{n}$, exhibiting this texture corresponds to a serpentine profile along the prior shearing direction [2, 3, 6]. Recently, several investigators [7, 10, 12, 13] reported the idea of stored elastic energy as the internal driving force for transient and spatially periodic director reorientation. Despite being well-characterized, however, no definite explanation has yet been reported on the mechanism of the transient banded texture formation after cessation of shear flow [8, 12, 13]. The objective of this preliminary communication is to present a viscoelastic model that describes the mechanism of the transient banded texture formation after cessation of simple shear flow for a characteristic uniaxial rigid rod nematic polymer. Other complex banded textures formed during shear flows [1] are beyond the scope of this work.

The phenomenon is best described using Cartesian coordinates with the transient one dimensional planar director field represented by $\mathbf{n}(x,t)=(\cos\theta,\sin\theta,0)$, and the transient one dimensional reorientation-induced velocity field by $\mathbf{v}(x,t)=(0,u,0;$ x represents the prior shearing direction. The governing equations for the scalar order parameter s, which is a measure of the degree of molecular alignment along the director, and the director and velocity fields are obtained using a simplified version of a recent theory proposed by Ericksen that is applicable to nematic polymers [15, 16]. For

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simplicity, all the viscosities are assumed to be constants since they do not vary significantly with s [17]. The evolution equations for s and $\mathbf{n}$ are then expressed as

$$\dot{s} = -\frac{1}{\beta_1}\frac{\delta F_d}{\delta s} - \frac{\beta_2}{\beta_1}\mathbf{n}^T \cdot \mathbf{A} \cdot \mathbf{n}, \tag{1}$$

$$\dot{\mathbf{n}} = \boldsymbol{\Omega} \cdot \mathbf{n} + \frac{\gamma_2}{\gamma_1}[\mathbf{n}(\mathbf{n}^T \cdot \mathbf{A} \cdot \mathbf{n}) - \mathbf{A} \cdot \mathbf{n}] - \frac{1}{\gamma_1}\frac{\delta F_d}{\delta \mathbf{n}}, \tag{2}$$

where β_1, β_2, γ_1 and γ_2 are viscosities. The superposed dot denotes the material time derivative, and $\delta/\delta q$ denotes the functional derivative with respect to q. The kinematic quantities are defined as follows: $\mathbf{A} = [(\nabla \mathbf{v})^T + \nabla \mathbf{v}]/2$, $\boldsymbol{\Omega} = [(\nabla \mathbf{v})^T - \nabla \mathbf{v}]/2$, and $\nabla \mathbf{v}$ is the velocity gradient. The free energy density, F_d, is given as [18, 19]

$$F_d = F_0(T) + k_B \vartheta T[\tfrac{1}{2}(1 - \tfrac{1}{3}U)s^2 - \tfrac{1}{9}Us^3 + \tfrac{1}{6}Us^4] + \tfrac{1}{2}K_5(\nabla s)^2 + \tfrac{1}{2}K_6(\mathbf{n} \cdot \nabla s)^2 + \tfrac{1}{4}Ks^2$$
$$\times [(\nabla \cdot \mathbf{n})^2 + (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 (\mathbf{n} \times \nabla \times \mathbf{n})^2] + 2K_6 s(\nabla \cdot \mathbf{n}) \times (\mathbf{n} \cdot \nabla s) + K_6 s(\mathbf{n} \times \nabla \times \mathbf{n}) \cdot \nabla s, \tag{3}$$

where $F_0(T)$, k_B, ϑ, T, U and K_i's are the isotropic free energy, Boltzmann constant, rod concentration, temperature, nematic potential and elastic constants, respectively. For simplicity, Frank elastic isotropy is assumed in equation (3). The linear momentum balance equation for an incompressible fluid under creeping flow and no external body forces reduces to

$$\nabla \cdot \boldsymbol{\tau} = 0, \tag{4}$$

where $\boldsymbol{\tau}$ is the stress tensor expressed as [20]

$$\boldsymbol{\tau} = -p\boldsymbol{\delta} - \frac{\partial F_d}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T + \alpha_1(\mathbf{nn} : \mathbf{A})\mathbf{nn} + \alpha_2 \mathbf{nN}$$
$$+ \alpha_3 \mathbf{Nn} + \alpha_4 \mathbf{A} + \alpha_5 \mathbf{nn} \cdot \mathbf{A} + \alpha_6 \mathbf{A} \cdot \mathbf{nn}, \tag{5}$$

where p is the pressure, δ is the identity tensor, α_j's are the Leslie viscosities, and $\mathbf{N} = \dot{\mathbf{n}} - \boldsymbol{\Omega} \cdot \mathbf{n}$.

Equations (1), (2) and (4) are solved numerically along the prior shearing direction with the following initial and boundary conditions: at $t = 0$, $s = s_0 + A_s \sin(k_s \pi x + \phi)$, $\theta = A_\theta \sin(k_\theta \pi x + \phi)$, $u = 0$; and at $x = 0$ and at $x = L$, $\partial s/\partial x = 0, \partial \theta/\partial x = 0, u = 0$ using Galerkin finite elements, 252 linear elements and a first order implicit Euler predictor-corrector time integrator [21]. The Leslie viscosities used are for the nematic polymer poly(4,4′-dioxy-2,2′-dimethyl azoxybenzenedodecanediyl) [22]. Values for other parameters are as follows: $\beta_1 = 50\gamma_1$, $\beta_2 = -100\gamma_1$, $k_B \vartheta T = 1{\cdot}04 \times 10^3$ J m^{-3}, $U = 5{\cdot}769$, $K = K_5 = 3{\cdot}78 \times 10^{-11}$ N, $K_6 = 10K$, $s_0 = 0{\cdot}75$, $A_s = 0{\cdot}108$, $A_\theta = 0{\cdot}01$ rad, $k_s = 126/Lm^{-1}$, $k_\theta = 21/L\,\mathrm{m}^{-1}$, $\phi = \pi/2$ rad, and $L = 157{\cdot}5 \times 10^{-6}$ m. The value for k_s is chosen as such to represent a possible spatial fluctuation in s, since there are, to the author's knowledge, no experimental reports in the literature on how shear flow affects s spatially. The value for k_θ is chosen as such to result in a bright band width of $7{\cdot}5 \times 10^{-6}$ m, which is a typical value [1, 5, 6, 8, 9]. Furthermore, it will be shown in a future paper that this band width is the fastest growing one when compared to larger and smaller widths according to the principle that the fastest growing width optimizes the effects due to elasticity and backflows [23, 24].

Figure 1 shows the time evolution of the dimensionless spatial distributions of s (upper row), θ (middle row) and the dimensionless velocity u^* (bottom row) at $t = 0{\cdot}0$ s (left column: initial state), $t = 19{\cdot}8$ s (middle column: banded texture formation stage)

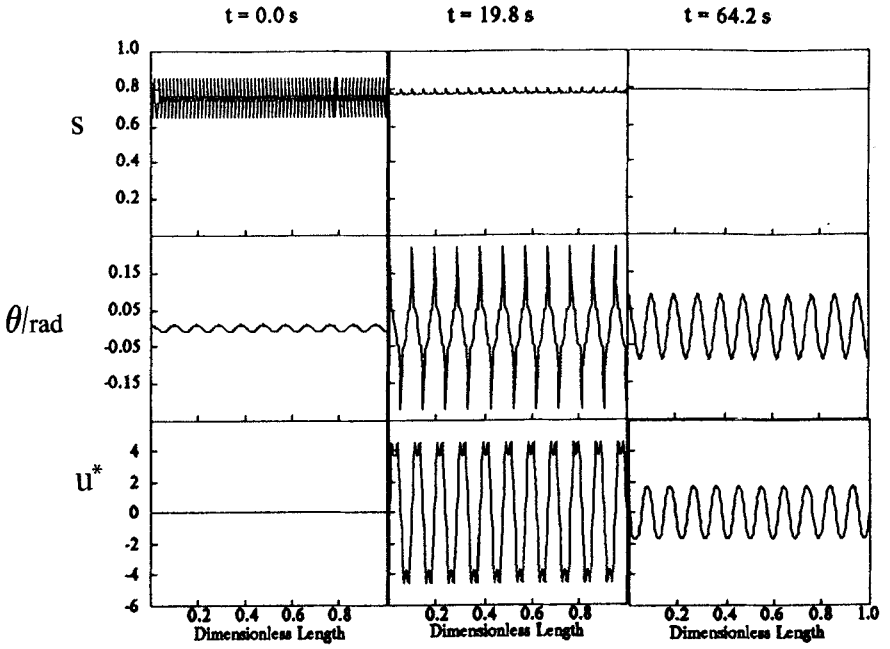

Figure 1. Time evolution of the dimensionless spatial distributions of the scalar order parameter s, orientation angle θ and the dimensionless velocity u^* at $t=0{\cdot}0$ s (left column: initial state), $t=19{\cdot}8$ s (middle column: banded texture formation stage), and $t=64{\cdot}2$ s (right column: banded texture relaxation stage), respectively. The scales are given by $u^*=uL\gamma_1/K$ and $x^*=x/L$.

Figure 2. A one and a half wavelength of the digitized optical pattern, representing the pattern seen between crossed polars at 19·8 s. The relative maximum intensity is white and the relative minimum is black.

and 64·2 s (right column: banded texture relaxation stage); the scales are given by $u^*=uL\gamma_1/K$ and $x^*=x/L$. The initial state of s represents the shear-flow enhanced fluctuations nematic polymers are expected to have during flow [17]. The notion of spatially non-homogeneous scalar order parameter is further supported by the predicted periodic oscillations of s in monodomain and spatially invariant nematic polymer systems during shear flow [25, 26]. While these fluctuations in s relax, they produce spatially periodic torques on the director (19·8 s) and the stored elastic energy decays; this is mainly due to the couplings between $\mathbf{n}$ and ∇s introduced by the K_6 constant in equation (3). As the fluctuations continue to decay, so do the driving torques and the director begins to reorient towards its initial state (64·2 s). The response is viscoelastic since periodic reorientation creates periodic backflows, as shown in the bottom row of figure 1. The maximum orientation angle of 0·2 rad at $t=19{\cdot}8$ s within the range of experimentally measured values [1, 2, 5, 6, 9, 14].

The digitized optical pattern representing the pattern seen between crossed polars at 19·8 s for one and a half wavelengths is shown in figure 2, where the relative intensity is calculated using $I = I_0 \sin^2(2\theta)$ [27]. A strong resemblance should be noted between this pattern and the banded texture shown in the literature referenced above.

This model demonstrates that the relaxation of stored elastic energy due to periodic fluctuations in the scalar order parameter results in a transient periodic distortion of the director field, such that a banded texture is seen when the sample is viewed between crossed polars. A detailed report on the results from this model will be given very shortly.

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