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Programmed shape of glassy nematic sheets with varying in-plane director fields: A kinetics approach

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ABSTRACT

Programmed deformation of glassy nematic sheets with continuously varying in-plane director fields is studied using Föppl-von Kármán plate theory. To solve the nonlinear governing equations, an efficient kinetics approach is developed, in which the deformed shape of a sheet can be recovered from the steady-state solution of an overdamped evolution system driven by elastic energy release. Numerical examples are given for circular nematic sheets with two kinds of director alignment. It is found that the director pattern, the radius-to-thickness ratio, and the elastic anisotropy along and normal to the director all can strongly influence the buckling morphologies. These results are important to the exploration of encoding three-dimensional shapes using glassy nematic sheets.

1. Introduction

Nematic glasses and elastomers are cross-linked liquid crystal polymer networks. These materials respond to heating or illumination with reversible contraction along and expansion normal to the director (Finkelmann et al., 2001; Hogan et al., 2002; Yu et al., 2003; van Oosten et al., 2007), thus are very promising in a variety of applications including actuation (van Oosten et al., 2009; Modes et al., 2013; Smith et al., 2014; Yang and He, 2014) and shaping (McConney et al., 2013; de Haan et al., 2014; White and Broer, 2015; Ware et al., 2015). Recent progress in synthesis technology enables precise inscription of various director alignments (de Haan et al., 2012; Ware et al., 2015). This offers the possibility of programming the deformation of nematic solids by engineering the director fields (Fuchi et al., 2015; Modes and Warner, 2016; Plucinsky et al., 2016).

We are concerned here with nematic glasses. The high cross-linking density causes the material to possess elastic modulus as high as a few gigapascals, and the director within it is not independently mobile from the elastic matrix as it is in elastomers (van Oosten et al., 2007). There has been great effort made to quantify the influence of director alignment on the deformation of glassy nematic sheets. The early studies were focused mainly on splay-bend and twist distributions, and the classical plate theory was extended to account for the spontaneous strains caused by light or heating. Along this line, analytical solutions were obtained for the deformed shapes of some free-standing and constrained sheets with simple geometries (Warner et al., 2010a; He, 2013). The effect of elastic anisotropy was examined (Modes et al., 2010a; He and Huang, 2014), and the phenomena of curvature suppression (Warner et al., 2010b) and bifurcation (He, 2014) were also analyzed in the scope of large deflections. Recently, increasing attention has been paid to nematic sheets with more diverse in-plane director patterns. The key is to design director fields which lead to proper inhomogeneous in-plane stress distributions and further create some desired buckling shapes. To establish quantitative links between director patterns and programmed morphologies, the sheets are assumed sufficiently thin so that they can purely bend at no stretch energy cost. Therefore, the deformation is an isometric immersion of the metric determined by the director field. Following such a routine, emergent morphologies of the sheets arising from differently charged topological defects and their textures were predicted (Modes et al., 2010b; Modes and Warner, 2011; Zakharov and Pismen, 2015; Mostajeran, 2015; Mostajeran et al., 2016), and the reverse problem of constructing a director field which induces a specified shape was also explored (Aharoni et al., 2014). Despite the successes, however, the method adopted in these researches possesses an obvious shortcoming of missing the role played by the elastic moduli of the sheet. An immediate consequence is that possible multi-stable configurations (He, 2014) arising from the competition between bending and stretch of the nematic sheets cannot be well reflected.

In this paper, we attempt to propose a general model for the deformation of glassy nematic sheets. Both effects of continuously varying in-plane director orientation and material anisotropy are considered, and large deflections are incorporated in the scheme

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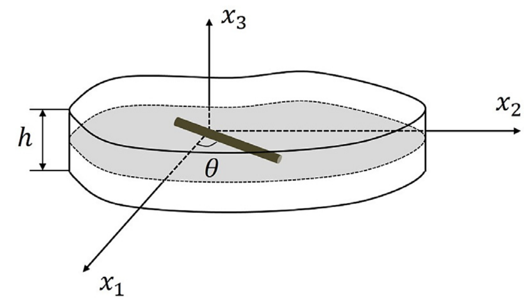

Fig. 1. Sketch of a glassy nematic sheet with varying in-plane director orientation.

of the Föppl-von Kármán plate theory. To solve the resulting nonlinear differential equations with variable coefficients, we treat the nematic sheets as overdamped evolution systems driven by elastic energy release according to Ginzburg-Landau kinetic equation. Therefore the equilibrated morphologies of the sheets can be determined once the steady-state solutions of the system are obtained. To demonstrate the application of the approach, numerical examples are given for circular nematic sheets with two kinds of director fields. The effect of elastic anisotropy, which is inherent to nematic solids, is examined. Our results indicate that the deformed shapes depend not only on the director pattern, but also on the ratio of radius to thickness and the elastic anisotropy.

2. Theoretical formulation

We start with considering a finite and arbitrarily shaped glassy nematic sheet of constant thickness h. As shown in Fig. 1, a rectangular coordinate system (x_1,x_2,x_3) is introduced so that the mid-plane of the sheet lies in the x_1-x_2 plane. No external load is applied on the top and bottom surfaces, and the lateral edge of the sheet may be free or fully clamped. The director orientation within the sheet does not change across the thickness, but may exhibit any smooth variation in the x_1-x_2 plane. Thus the director field can be characterized by a unit vector $\mathbf{n}=(n_1,n_2,0)$, where $n_1=cos\theta$, $n_2=sin\theta$, and $\theta=\theta(x_1,x_2)$ is the angle between the director and the x_1-axis. Upon illumination or heating, spontaneous contraction $\varepsilon_\parallel$ and expansion $\varepsilon_\perp$ occur in the directions along and normal to $\mathbf{n}$, respectively, thereby causing deformation of the sheet. We will formulate a model to predict such a deformation based on the Föppl-von Kármán plate theory. For convenience, the usual summation convention for repeated subscripts is adopted, in which Latin subscripts run from 1 to 3 while Greek ones take values of 1 or 2. A comma means differentiation with respect to the suffix coordinate.

The spontaneous contraction and expansion lead to a spontaneous strain field $\varepsilon^*_{ij}=\varepsilon^*_{ij}(x_1,x_2)$ of the form

$$\varepsilon^*_{ij}=(\varepsilon_\parallel-\varepsilon_\perp)n_in_j+\varepsilon_\perp\delta_{ij} \tag{1}$$

where δ_{ij} is Kronecker's delta which equals 1 for $i=j$ and vanishes otherwise. In general, the magnitudes of $\varepsilon_\parallel$ and $\varepsilon_\perp$ may be not constant due to their dependence on local light intensity and temperature rise (van Oosten et al., 2007). Yet, we constrain ourselves here to the case that the sheet is uniformly illuminated or heated, so that $\varepsilon_\parallel$ and $\varepsilon_\perp$ are viewed as constants. More complex situation for varying $\varepsilon_\parallel$ and $\varepsilon_\perp$ with position can be treated in the same way. Locally, the nematic sheet reveals transversely isotropic elasticity about $\mathbf{n}$, and needs to be described by five independent material constants (Modes et al., 2010a). A compact representation for the stress-strain relation of the sheet is given by (Spencer, 1982),

$$\begin{aligned}\sigma_{ij}&=\lambda(\varepsilon_{kk}-\varepsilon^*_{kk})\delta_{ij}+2\mu(\varepsilon_{ij}-\varepsilon^*_{ij})\\&\quad+\alpha\left[n_kn_l(\varepsilon_{kl}-\varepsilon^*_{kl})\delta_{ij}+n_in_j(\varepsilon_{kk}-\varepsilon^*_{kk})\right]\\&\quad+2(\mu_0-\mu)\left[n_in_k(\varepsilon_{kj}-\varepsilon^*_{kj})+n_jn_k(\varepsilon_{ki}-\varepsilon^*_{ki})\right]\\&\quad+\beta n_in_jn_kn_l(\varepsilon_{kl}-\varepsilon^*_{kl})\end{aligned} \tag{2}$$

where σ_{ij} and ε_{ij} are components of stress and strain tensors respectively, and λ, μ, μ_0, α and β are five elastic constants. Expressions of these constants in terms of the engineering stiffness coefficients in Voigt notation as well as in terms of Young's moduli, Poisson's ratios and shear modulus are provided in Appendix A. The normal stress σ_{33} in the sheet is much smaller in magnitude than the other stress components and is negligible. Using this condition in Eq. (2) yields

$$\varepsilon_{33}-\varepsilon^*_{33}=-\frac{1}{\lambda+2\mu}(\lambda\delta_{\alpha\beta}+\alpha n_\alpha n_\beta)(\varepsilon_{\alpha\beta}-\varepsilon^*_{\alpha\beta}) \tag{3}$$

Therefore, substituting the above result back into Eq. (2), we arrive at the reduced stress-strain relation

$$\begin{aligned}\sigma_{\alpha\beta}&=\Lambda_{\alpha\beta\omega\rho}(\varepsilon_{\omega\rho}-\varepsilon^*_{\omega\rho})\\\sigma_{\alpha3}&=2\left[\mu\delta_{\alpha\beta}+(\mu_0-\mu)n_\alpha n_\beta\right]\varepsilon_{\beta3}\end{aligned} \tag{4}$$

in which $\Lambda_{\alpha\beta\omega\rho}=\Lambda_{\omega\rho\alpha\beta}=\Lambda_{\beta\alpha\omega\rho}=\Lambda_{\alpha\beta\rho\omega}$ are the reduced in-plane elastic constants defined by

$$\begin{aligned}\Lambda_{\alpha\beta\omega\rho}&=2\mu\delta_{\alpha\omega}\delta_{\beta\rho}+\frac{2\mu}{\lambda+2\mu}\left(\lambda\delta_{\alpha\beta}\delta_{\omega\rho}+\alpha\delta_{\alpha\beta}n_\omega n_\rho+\alpha\delta_{\omega\rho}n_\alpha n_\beta\right)\\&\quad+2(\mu_0-\mu)\left(\delta_{\alpha\rho}n_\beta n_\omega+\delta_{\beta\rho}n_\alpha n_\omega\right)\\&\quad+\left(\beta-\frac{\alpha^2}{\lambda+2\mu}\right)n_\alpha n_\beta n_\omega n_\rho\end{aligned} \tag{5}$$

Obviously, $\Lambda_{\alpha\beta\omega\rho}$ are functions of the in-plane coordinates x_1 and x_2.

For thin nematic sheets, the transverse shear deformation is negligible so that the displacement u_i at any point can be assumed as

$$u_\alpha=u^0_\alpha-x_3w_{,\alpha}\qquad u_3=w \tag{6}$$

where u^0_α and w are respectively the in-plane and out-of-plane displacement components of the mid-plane. Then the only nonzero strains in the Föppl-von Kármán sense read $\varepsilon_{\alpha\beta}=\varepsilon^0_{\alpha\beta}-x_3w_{,\alpha\beta}$, in which

$$\varepsilon^0_{\alpha\beta}=\frac{1}{2}(u^0_{\alpha,\beta}+u^0_{\beta,\alpha})+\frac{1}{2}w_{,\alpha}w_{,\beta} \tag{7}$$

The corresponding stresses are

$$\sigma_{\alpha\beta}=\Lambda_{\alpha\beta\omega\rho}(\varepsilon^0_{\omega\rho}-\varepsilon^*_{\omega\rho}-x_3w_{,\omega\rho}) \tag{8}$$

and the membrane forces $N_{\alpha\beta}$ and moments $M_{\alpha\beta}$, defined by

$$N_{\alpha\beta}=\int_{-h/2}^{h/2}\sigma_{\alpha\beta}dx_3\qquad M_{\alpha\beta}=\int_{-h/2}^{h/2}\sigma_{\alpha\beta}x_3dx_3 \tag{9}$$

can be obtained as

$$\begin{aligned}N_{\alpha\beta}&=A_{\alpha\beta\omega\rho}(\varepsilon^0_{\omega\rho}-\varepsilon^*_{\omega\rho})\\M_{\alpha\beta}&=-D_{\alpha\beta\omega\rho}w_{,\omega\rho}\end{aligned} \tag{10}$$

with

$$A_{\alpha\beta\omega\rho}=\Lambda_{\alpha\beta\omega\rho}h\qquad D_{\alpha\beta\omega\rho}=\frac{1}{12}\Lambda_{\alpha\beta\omega\rho}h^3 \tag{11}$$

With these results, the total energy of the sheet is expressed by

$$U=\frac{1}{2}\int_A\left[N_{\alpha\beta}\left(\varepsilon^0_{\alpha\beta}-\varepsilon^*_{\alpha\beta}\right)-M_{\alpha\beta}w_{,\alpha\beta}\right]dA \tag{12}$$

where A is the area of the mid-plane. Minimization of U with respect to u^0_α and w requires

$$\begin{aligned}N_{\alpha\beta,\beta}&=0\\M_{\alpha\beta,\alpha\beta}+N_{\alpha\beta}w_{,\alpha\beta}&=0\end{aligned} \tag{13}$$

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