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Mechanical frustration and spontaneous polygonal folding in active nematic sheets

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We analyze the bending response to light or heat of a solid nematic disk with a director twisted from being radial on the upper surface to be azimuthal on the lower. We find a number of curl lobes determined purely by the geometry of the mechanical frustration that arises during the response.

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Nematic glasses and elastomers contract along their director $\underline{n}$ by a factor λ (<1) and elongate by a factor $\lambda_\perp$ (>1) perpendicular to $\underline{n}$ when their order is reduced. Heat, or illumination if dye molecules are present, drive this order change and hence mechanical response. Recovery occurs on cooling or in the dark. Bend occurs if there is a gradient of light intensity through the thickness of the cantilever (due to light absorption as the dye is stimulated) [1].

Mechanical frustration arises as it does in classical bend due to Poisson effects which induce saddle shapes for small deflections. As one bend increases, bend in the other direction induces unavoidable stretch as elements are deflected far from the neutral plane. Such a stretch is inherently much more costly than the simple bends by themselves. A classic example is trying to bend a builder's tape measure backward in the face of its natural bend in the transverse direction.

The result in classical beams and metal tape measures is the suppression of bend in one direction to lower the cost of bend in the other. One can think of this as a geometric-mechanical form of frustration.

Complex director distributions in nematic solids can cause more complex bends and twists [1–3], but also still further exacerbate frustration. We have created solid nematic disks with a radial in-plane director on one face, twisting to being azimuthal on the other, and term such distributions "radimuthal." Such radial or azimuthal fields, on heating or illumination, are separately known [4–6] to produce Gaussian curvature localized at the disk center, in the form of cones or anticones. Remarkably stretch is avoided, though there is some lower bend energy. However, it is far from clear how a radimuthal disk should bend on heating (or illumination) since there are competing effects. A simpler example we also use in constructing the bend energy of the disk is that of a cantilever also with an $\underline{n}$ twisted through its thickness from being longitudinal on one face to perpendicular on the other [see Fig. 1(b)]. Contraction by a factor of λ along y at the top face and elongation by $\lambda_\perp$ along y at the bottom (with varying degrees of this at various depths) naturally gives bend in the y-z plane. But equally, elongation by $\lambda_\perp$ along x at the top face and contraction λ along x at the bottom gives an equal and opposite bend in the x-z plane and a perfect saddle (anticlastic surface) should result [see Fig. 1(a)]. This (negative) Gaussian curvature gives stretch and the x-z bend is ultimately suppressed when the y-z deflection becomes large. See Ref. [7] for suppression in nematic cantilevers—an equivalent of the classical Love problem [8] of curvature suppression in conventional elasticity.

When a director is at angle θ to the x axis, the natural x,y distortions the system would like to achieve in response to light are given by

$$\underline{\underline{\lambda}} = \begin{pmatrix} \lambda_\perp + \Delta\lambda c_\theta^2 & \Delta\lambda s_\theta c_\theta \\ \Delta\lambda s_\theta c_\theta & \lambda_\perp + \Delta\lambda s_\theta^2 \end{pmatrix} \equiv \begin{pmatrix} \lambda_{xx} & \lambda_{xy} \\ \lambda_{yx} & \lambda_{yy} \end{pmatrix}, \quad (1)$$

where $\Delta\lambda = \lambda - \lambda_\perp$, $c_\theta = \cos\theta$, $s_\theta = \sin\theta$, and $\theta = \pi/4 + \pi z/(2h)$ through the thickness $z = -h/2 \to h/2$. There is in addition a natural zz distortion of $\lambda_\perp$. However, in this twisted $\underline{n}(z)$ system, contraction along the different $\underline{n}(z)$ at different depths z would cause enormous shears and thus distortion so varying with depth is suppressed. An approximate (neglecting coupling to λ_{zz}), homogeneous, energy-reducing distortion would be $\overline{\lambda}_{xx} = \overline{\lambda}_{yy} = (\lambda + \lambda_\perp)/2$. The energy cost per unit area U, associated with adopting this mean xx distortion rather than individually optimal values appropriate at each depth z, is

$$U = \frac{1}{2} G \int_{-h/2}^{h/2} dz \left[\overline{\lambda}_{xx} - \lambda_\perp - \Delta\lambda \cos^2\left(\frac{\pi}{4} + \frac{\pi z}{2h}\right)\right]^2 = \frac{1}{2} G \frac{(\Delta\lambda)^2}{8} h, \quad (2)$$

with G a modulus; see Refs. [1,2] for more details of calculations for cantilevers with complex director distributions. This energy per unit area associated with λ_{xx} assumes small strains $\lambda \sim \lambda_\perp \sim 1$. The equivalent yy energy also arises, along with analogous energies from the suppression of some of the shears in Eq. (1).

Take now in addition to just the mean distortion a yz bend with radius of curvature R_c giving a distortion of $\lambda_{xx} = \overline{\lambda}_{xx} - z/R_c$. The energy cost per unit area of not attaining the locally optimal distortion is instead (simplifying λ terms and using a

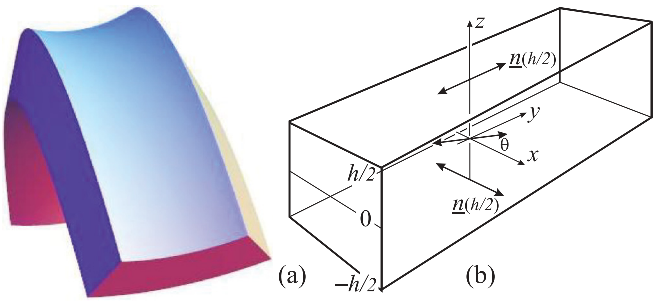

FIG. 1. (Color online) (a) Bend in two orthogonal directions and of opposite sign gives rise to a saddle shape. (b) A cantilever with a twisted nematic director distribution through its thickness.

double angle result)

$$U = \frac{1}{2}G\int_{-h/2}^{h/2} dz\left[-\frac{\Delta\lambda}{2}\cos\left(2\alpha+\frac{\pi}{2}+\frac{\pi z}{h}\right)-z/R_c\right]^2$$
$$= \frac{1}{2}Gh\left(\frac{(\Delta\lambda)^2}{8}+\frac{h^2}{12R_c^2}+\frac{h\Delta\lambda}{R_c}\frac{2}{\pi^2}\cos(2\alpha)\right). \quad (3)$$

We have allowed for an offset angle α of $\underline{n}(h/2)$ at the top face away from its being longitudinal with the cantilever; consider $\alpha = 0$ for the moment, i.e., the $\underline{n}(z)$ of Fig. 1. The elastic energy is reduced by bend from its value (2) in the flat state: $dU/d(h/R_c) = 0$ yields

$$h/R_c = -\frac{12}{\pi^2}\Delta\lambda, \quad U_{\rm min} = \frac{1}{2}Gh(\Delta\lambda)^2\left(\frac{1}{8}-\frac{24}{\pi^4}\right). \quad (4)$$

This beam is frustrated in that the x and y directions are equivalent, but both cannot bend since the two bends simultaneously would give Gaussian curvature and hence stretch, which is much higher in energy.

Now consider the disk, of radius R, with the radimuthal $\underline{n}(\underline{r})$. We term it the radimoid. Radial sections in Fig. 2 resemble the twist cantilevers of Fig. 1, with a longitudinal (radial) director on the top surface, and a transverse (azimuthal) director below. But to relieve the energy cost of remaining flat, curling can only be in one direction collectively if there is to be no stretch. Alternatively the radimoid divides into sectors, with part of each sector curling in its own unique

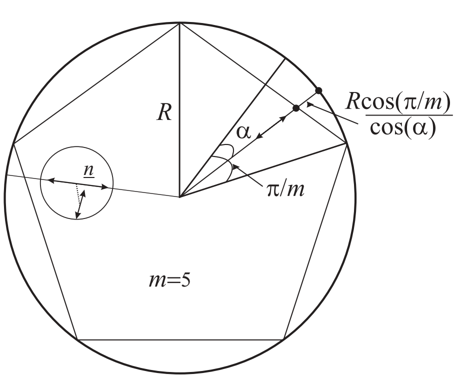

FIG. 2. A flat radimoid becoming a five-sector disk on curling. A schematic (circled) shows the director twisting radial (top surface) to azimuthal (bottom). The part at angle α to the bisector that will curl along the sector's bisector takes radial values between $R\cos(\pi/m)/\cos\alpha$ and R.

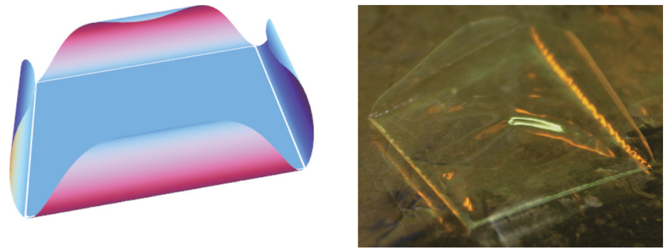

FIG. 3. (Color online) Left: A curled up, four-sector radimoid. Right: An initially flat, circular, radimoidal sheet when heated curls up with four sectors.

direction [see Fig. 3 (left)], but at the cost of curling only in the small outer lips. In this mode of bending, a section at angle α to the middle of the sector is forced to bend at an angle α to its natural axis (see Fig. 2), unlike in cantilevers with uniform offset to their twist which can form twisted ribbons or helicoids [3]. The α part of the energy (2) is that linear in h/R_c and is thus the part leading to energy reduction in optimizing the bilinear form $(\cdots)(h/R_c)^2 + (\cdots)(h/R_c)$. At $\alpha = \pi/4$ the h/R_c term vanishes and thereafter for $\alpha > \pi/4$ there is actually an energy increase on bending for a sign of h/R_c determined by the majority of sections which have $\alpha \in (-\pi/4,\pi/4)$. These sections with high α are backbending against their natural bend. This analysis suggests the answer to our principal question: What is the optimal number of sectors into which a radmoid, with its bend frustration, must form? Clearly $|\alpha| \leqslant \pi/4$ and hence the number of sectors $m \geqslant 4$ is desirable so that all regions of bend lead to energy reduction. For $m = 2$ (the disk just rolling up along a diameter) and hence $\alpha \in (-\pi/2,\pi/2)$, energy reduction on bending for $|\alpha| \leqslant \pi/4$ is canceled by the increase associated with $|\alpha| > \pi/4$. On the other hand, for increasing m the area undergoing bend decreases so it is possible $m = 3$ could be optimal. But narrower sectors have more effective bend-inspired reductions in energy—smaller α in the h/R_c term of Eq. (3)—favoring $m = 5, \ldots$.

To obtain the total curling energy, the curling region of each sector has its bend energy per unit area of Eq. (3) integrated over and then we must multiply by the number of sectors:

$$U_{\rm curl} = m\int_{-\pi/m}^{\pi/m} d\alpha \int_{R\frac{\cos(\pi/m)}{\cos\alpha}}^{R} r\,dr \cdot [(3)]$$
$$= R^2 m\int_0^{\pi/m} d\alpha\left(1-\frac{\cos^2(\pi/m)}{\cos^2\alpha}\right)\cdot[(3)].$$

Performing the integrations trivially,

$$U_{\rm curl} = \frac{1}{2}GhR^2 m\left[\left(\frac{\pi}{m}-\frac{1}{2}s_{2\pi/m}\right)\left(\frac{(\Delta\lambda)^2}{8}+\frac{h^2}{12R_c^2}\right) - \frac{\Delta\lambda h}{R_c}\frac{4}{\pi^2}\left(\frac{\pi}{m}c_{\pi/m}^2-\frac{1}{2}s_{2\pi/m}\right)\right]. \quad (5)$$

Optimizing over h/R_c, the reduced sector curvature, that is, $dU_{\rm curl}/d(h/R_c) = 0$, one obtains

$$\frac{h}{R_c} = \frac{24\Delta\lambda}{\pi^2}\frac{\frac{\pi}{m}c_{\pi/m}^2-\frac{1}{2}s_{2\pi/m}}{\frac{\pi}{m}-\frac{1}{2}s_{2\pi/m}}, \quad (6)$$

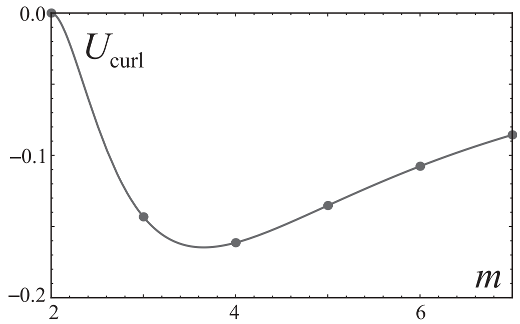

FIG. 4. Energy reduction due to bend against sector number m. The line is of the geometric (purely m-dependent) part of Eq. (7), with physical meaning for integers (dotted). The optimal number of sectors for an illuminated radimoid is 4.

which indeed vanishes for $m = 2$. Returning the optimal curvature to Eq. (5) and ignoring the reference energy $\sim(\Delta\lambda)^2/8$ associated with the average, shear-avoiding strain response through the thickness—which occurs all over the radimoid in equal measure, both curled and flat sections alike—the energy reduction is

$$U_{\rm curl} = -\frac{1}{2} G\pi R^2 h(\Delta\lambda)^2 \frac{48}{\pi^5} m \frac{\left(\frac{\pi}{m} c^2_{\pi/m} - \frac{1}{2} s_{2\pi/m}\right)^2}{\left(\frac{\pi}{m} - \frac{1}{2} s_{2\pi/m}\right)}. \quad (7)$$

The first part of (7) is the volume of the whole disk times an energy per unit volume of $\frac{1}{2}G(\Delta\lambda)^2$ characteristic of the anisotropy of the distortion not being achieved, times $48/\pi^5$, which reflects the depth variation of the direction of anisotropy and thus the extent to which the bend only partially relieves this elastic energy. The remaining factor, purely dependent on sector number m, is geometric. Figure 4 shows that the geometric part of the energy reduction due to bend is greatest at $m = 4$, as suspected. But the $m = 3$ and 5 states are relatively close in energy and could instead be achieved if there were imperfections, deviations from circularity, etc., or simply if the radimoid settled into a metastable basin of the energy landscape.

By using opposing plates with azimuthal and radial alignment layers on them, the reactive liquid crystalline mixture adopts a twisted nematic texture going through the thickness which is then made permanent by crosslinkage into a glass. Methods of creating such plates and solid sheets are described in earlier work [6]. Figure 3 (right) shows such a sheet heated and indeed forming a 4-lobe curled up structure.

Summary. A twist director field through the thickness of a solid nematic disk yields distortions even more frustrated than in classical bend elasticity. We calculate the energy and show that the optimal symmetry-breaking pattern of distortion depends purely on geometry. Competing states exist close to the four-sector optimal result and the experimental answer could be critically effected by imperfections. The extent of curling depends on the anisotropy of the natural response along and perpendicular to the director, $\Delta\lambda = \lambda - \lambda_\perp$, which would result when there are no constraints or mechanical frustration. Changing from heating to cooling (or from illumination to darkness) reverses the role of the director and directions perpendicular to it. Since the radimoid has both directions equally represented, cooling would see the same lobes produced, but curling down rather than up.

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