Numerical Experiments for Thermally-induced Bending of Nematic Elastomers with Hybrid Alignment (HNEs)

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Details on the actual experiment can be found in:

Y. Sawa, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi, *Thermally Driven Giant Bending of Liquid Crystal Elastomer Films with Hybrid Alignment*. **Macromolecules** 43, 4362–4369 (2010)

This paper received the **Outstanding Paper Award** in 2011 from the **Japanese Liquid Crystal Society**.

Nematic Elastomers with Hybrid Alignement (HNEs)

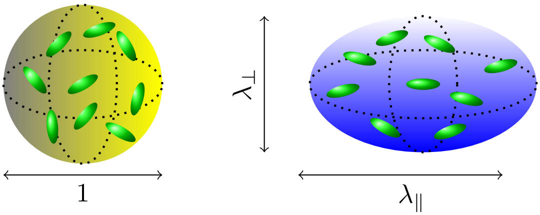


Figure: Mesoscopic chunk of NEs: disordered, isotropic phase (left); ordered, nematic phase (right). NE molecules are caricatured grossly out of scale.

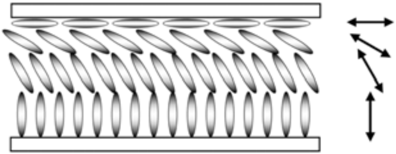


Figure: Schematic of hybrid orientation.

Experimental facts 1: nematic-isotropic phase transition

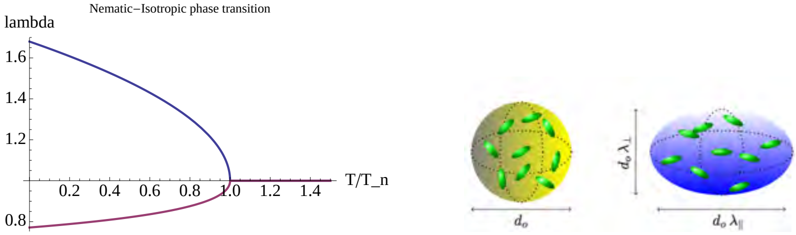


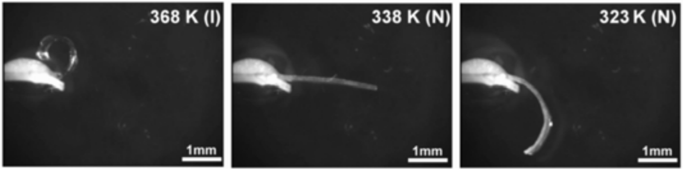
Figure: Effects of temperature on a mesoscopic chunk of NEs.

The elastomeric *distortions* we deal with are *uniaxial stretches* aligned with mesogen orientation $\mathbf{N}$:

$$\mathbf{U}_o = \lambda_{\parallel}\,\mathbf{N} + \lambda_{\perp}\,(\mathbf{I} - \mathbf{N})\,.$$

Experimental facts 2: rod-like specimen made of hybrid NEs

Macromolecules, vol. 43, pp. 4362–4369 (2010).



- solvent evaporation at low temperature induces a non-isotropic de-swelling, which is accompanied by a large bending (right);
- increasing the temperature, the macroscopic effects of the nematic phase decrease and a flat state is recovered (center);
- above the transition temperature the material is isotropic, and bending is very high, but in the opposite direction (left).

State diagram showing the phase transitions

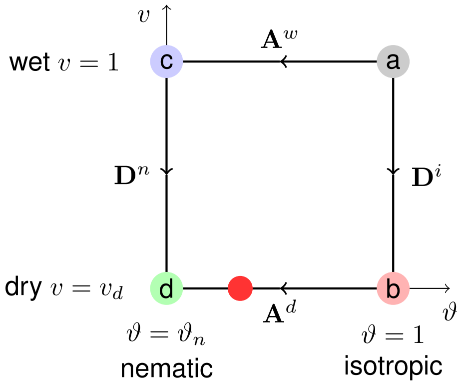


Figure: State diagram showing the phase transitions we consider. The goal is to model deswelling from (c) to (d); then, the temperature-driven phase transition nematic-isotropic, (d) to (b).

Representing the distortions

The distortions $\mathbf{D}^n(v)$ and $\mathbf{A}^d(\vartheta)$ are uniaxial stretches, sharing a same representation formula; here, we shall denote with $\alpha(v)$ and $\lambda(\vartheta)$ the swelling- and temperature-induced stretches, respectively:

$$\begin{aligned} \mathbf{D}^n(v) &= \alpha_{\|}(v)\,\mathbf{N} + \alpha_{\perp}(v)\,(\mathbf{I}-\mathbf{N})\,, \\ \mathbf{A}^d(\vartheta) &= \lambda_{\|}(\vartheta)\,\mathbf{N} + \lambda_{\perp}(\vartheta)\,(\mathbf{I}-\mathbf{N})\,, \end{aligned} \tag{1}$$

A distortion from point (c) to a generic state (ϑ, v) is described by the map $\bar{\mathbf{F}}_o$, which admits a straightforward representation

$$\bar{\mathbf{F}}_o(\vartheta, v) = \frac{\lambda_{\|}(\vartheta)\,\alpha_{\|}(v)}{\lambda_{\|}(\vartheta_n)}\,\mathbf{N} + \frac{\lambda_{\perp}(\vartheta)\,\alpha_{\perp}(v)}{\lambda_{\perp}(\vartheta_n)}\,(\mathbf{I}-\mathbf{N})\,. \tag{2}$$

The stretch measure

The distorted state is a ground state: you pay to stretch from $\bar{\mathbf{F}}_o$

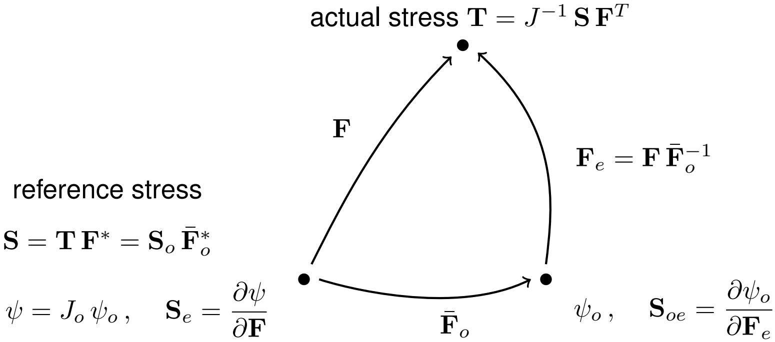


Figure: Stress measures and energy densities; $J = det(\mathbf{F})$.

The elastic energy

Let $\mathbf{F}$ denote a deformation with respect to the wet-nematic state (point c), and let $\mathbf{C} = \mathbf{F}^\top \mathbf{F}$ be the associated strain; the elastic deformation $\mathbf{F}^e$ and the elastic strain $\mathbf{C}^e$ are given by

$$\mathbf{F}^e = \mathbf{F}\,\bar{\mathbf{F}}_o^{-1}\,, \quad \mathbf{C}^e = (\mathbf{F}^e)^\top\,\mathbf{F}^e = \bar{\mathbf{F}}_o^{-\top}\mathbf{C}\,\bar{\mathbf{F}}_o^{-1}\,; \tag{3}$$

we consider a Neo-Hookean elastic energy density

$$\begin{aligned} &\phi = \tfrac{1}{2}\,\mu\,(\mathbf{C}^e \cdot \mathbf{I} - 3) = \tfrac{1}{2}\,\mu\,(\mathbf{C} \cdot \mathbf{C}_o^{-1} - 3)\,, \\ &\det(\mathbf{C}_o) = v^2, \end{aligned} \tag{4}$$

with μ the shear modulus; $\mathbf{C}_o$ is the distortional strain induced by $\bar{\mathbf{F}}_o$:

$$\mathbf{C}_o(\vartheta, v) = \bar{\mathbf{F}}_o^\top(\vartheta, v)\,\bar{\mathbf{F}}_o(\vartheta, v)\,. \tag{5}$$

The flat state

If $\mathbf{C}_o \propto \mathbf{I}$, we have a homogenous state, that is, a *flat* configuration. Moreover, the condition $\mathbf{C}_o = \bar{\mathbf{F}}_o^\top \bar{\mathbf{F}}_o \propto \mathbf{I}$ is equivalent to

$$\bar{\mathbf{F}}_o(\vartheta, v) = \frac{\lambda_{\|}(\vartheta)\,\alpha_{\|}(v)}{\lambda_{\|}(\vartheta_n)}\,\mathbf{N} + \frac{\lambda_{\perp}(\vartheta)\,\alpha_{\perp}(v)}{\lambda_{\perp}(\vartheta_n)}\,(\mathbf{I} - \mathbf{N}) =\propto \mathbf{I}\,. \tag{6}$$

It follows that ϑ_f satisfies

$$\frac{\lambda_{\|}(\vartheta_f)\,\alpha_{\|}^d}{\lambda_{\|}(\vartheta_n)} = \frac{\lambda_{\perp}(\vartheta_f)\,\alpha_{\perp}^d}{\lambda_{\perp}(\vartheta_n)}\,. \tag{7}$$

Actually, from experimental data [3], we know the deswelling distortions at the completely dry state, and the expressions relating the temperature to the cooling distortions,

The model implementation

We implement the balance equations of non-linear elasticity in weak form, using the volumetric-deviatoric decomposition of the deformation measures, and adopting a mixed method. We have as independent variables the displacement vector $\mathbf{u}$, and the pressure p; given $\mathbf{F} = \mathbf{I} + \nabla\mathbf{u}$, we consider the following relaxed strain energy density: $\phi_r = \phi_s + \phi_v$, with

$$
\begin{aligned}
\phi_s &= \tfrac{1}{2}\,\mu\,(\mathbf{C}_s \cdot \mathbf{C}_o^{-1} - 3) && \text{isochoric energy;}\\
\phi_v &= \tfrac{k}{2}\,(J - v)^2 && \text{volumetric energy;}\\
\mathbf{C}_s &= (v/J)^{2/3}\,\mathbf{C}\,, && \text{unimodular part of } \mathbf{C};\\
p &= -k\,(J - v)\,, && \text{pressure;}\\
J &= \det(\mathbf{F})\,, && \text{volume change;}
\end{aligned}
\tag{8}
$$

and k the bulk modulus.

Balance equations are implemented using a mixed L2-L1 method, that is using second- and first-order Lagrangian shape functions for the displacement and the pressure, respectively. The problem is then stated follows: find a displacement $\mathbf{u}$, and a pressure p such that, for all test function $\widetilde{\mathbf{u}}$, and $\widetilde{p}$ it holds:

$$\begin{aligned} &\int_B \big(-\mathbf{S} \cdot \nabla \widetilde{\mathbf{u}} + \mathbf{f} \cdot \widetilde{\mathbf{u}} \big) = 0\,, \\ &\int_B (\frac{p}{k} + J - v) \cdot \widetilde{p} = 0\,, \end{aligned} \tag{9}$$

with $\mathbf{u} = 0$ at $x = -L/2$. From our representation of the elastic energy, it follows that the reference stress is a function of the independent variables $\mathbf{u}$ and p, and of the state variables (ϑ, v):

$$\mathbf{S} = \mathbf{S}(\mathbf{u}, p; \vartheta, v)\,. \tag{10}$$

Nematic orientations

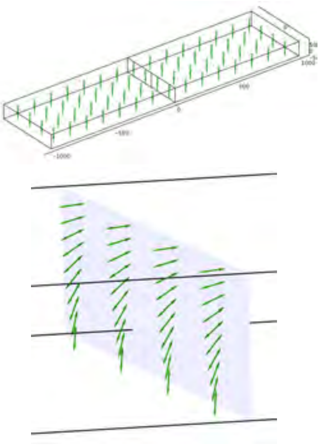


Figure: Whole specimen (top) and vertical cross section showing the nematic orientation (bottom).

Results 1

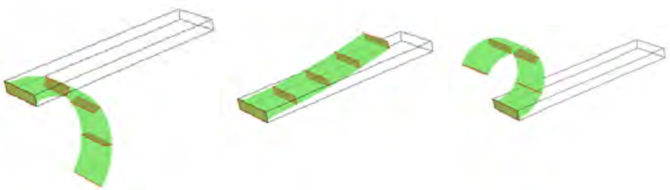


Figure: Results from numerical experiments. From top to bottom: dry state at preparation temperature ϑ_n; nearly flat state at $\vartheta \sim \vartheta_f$; isotropic state at $\vartheta = 1$. Wireframe renders the preparation state; five cross sections highlight bending.

Results 2

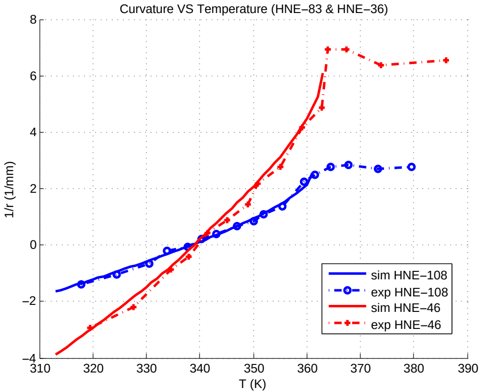


Figure: Curvature versus temperature. The plot shows the results from numerical (solid line) and actual (dotted line with marker) experiments for two similar specimens having different thickness and length ($H = 108 \sim 46\,\mu m$).

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