

Coupling between mass density and director arrangement in Nematic Liquid Crystals

Francesco dell'Isola^{2,3} Antonio DiCarlo^{1,3}
Giuseppe Rosi^{1,3} Luciano Teresi^{1,3}

¹LaMS - Modeling & Simulation Lab,
Università Roma Tre, Italy

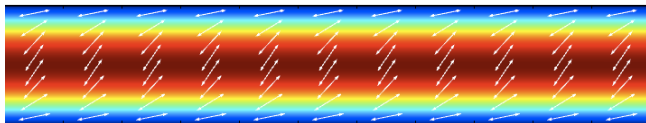
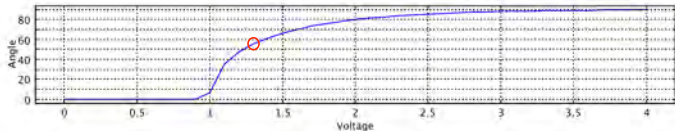
²Dipartimento di Ingegneria Strutturale e Geotecnica,
Università di Roma La Sapienza, Italy

³International Research Center on Mathematics and Complex Systems,
Università degli Studi dell'Aquila, Italy

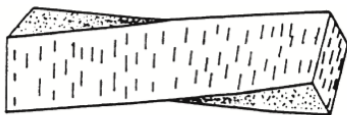
October 27th, 2011



Nematic Liquid Crystals and Freedericksz transition

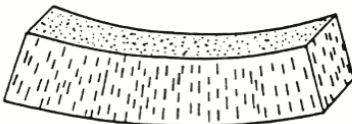


A NLC with strong anchoring conditions imposed at the boundaries shows an important bifurcation phenomenon which is known as Freedericksz transition



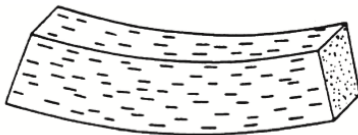
Twist

(a)



Splay

(b)

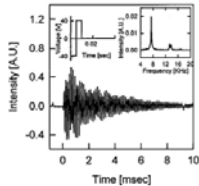


Bend

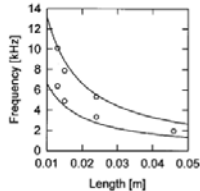
(c)

$$\begin{aligned}
 \psi_F = & \underbrace{\frac{1}{2}K_1 (\nabla \cdot \mathbf{n})^2}_{\text{Splay}} + \underbrace{\frac{1}{2}K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2}_{\text{Twist}} + \underbrace{\frac{1}{2}K_3 (\mathbf{n} \times \nabla \times \mathbf{n})^2}_{\text{Bend}} + \\
 & \underbrace{\frac{1}{2}(K_2 + K_4) \nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - (\nabla \cdot \mathbf{n}) \mathbf{n}]}_{\text{Saddle splay}}
 \end{aligned}$$

Y. Kim and J. Patel, " Acoustic generation in liquid crystals," Applied Physics Letters, vol. 75, p. 1985, 1999.



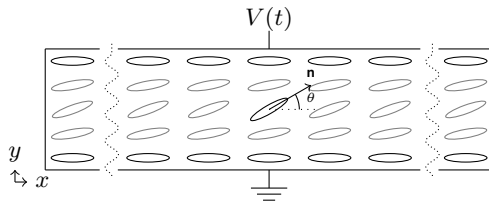
(a)



(b)

- (a) a pressure signal is detected only when the applied voltage exceeds the Freedericksz threshold
- (b) the frequency of the generated signal changes when modifying the dimensions of the sample

When driving the sample with an harmonic forcing signal at frequency f_o , a pressure field at $2f_o$ is detected.



The main characteristic of the proposed model are:

- Two dimensional problem
- Variable electric potential $V(t)$ applied on the top electrode
- Orientation waves must not be involved in the process of acoustic generation
- The mass density is coupled with the directors' orientation

The coupling between the directors' orientation and the density is based on the following considerations:

- when the directors of the nematic fluid are all parallel, then the molecules of the fluid are all packed in the most "ordered way" and the density of the liquid crystal attains its maximum value
- when close material particles of the liquid crystals have directors oriented in different directions the density varies depending on the assumed directors' configuration
- in presence of gradients of orientation, are more "loosely packed" and consequently the density is lower

The coupling term has this form:

$$\psi_I = \underbrace{\frac{1}{2}\alpha_1 (\nabla \cdot \mathbf{n})^2}_{\text{Splay}} + \underbrace{\frac{1}{2}\alpha_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2}_{\text{Twist}} + \underbrace{\frac{1}{2}\alpha_3 (\mathbf{n} \times \nabla \times \mathbf{n})^2}_{\text{Bend}} + \underbrace{\frac{1}{2}(\alpha_2 + \alpha_4)\nabla \cdot [(\mathbf{n} \cdot \nabla) \mathbf{n} - (\nabla \cdot \mathbf{n}) \mathbf{n}]}_{\text{Saddle splay}}$$



Four non-dimensional coupled equations in 2D

$$\Delta\theta - \frac{\pi^2}{2} \left[(\tilde{E}_x^2 - \tilde{E}_y^2) \sin 2\theta - \tilde{E}_x \tilde{E}_y \cos 2\theta \right] = 0 \quad \text{Balance of torques}$$

$$\nabla \cdot (\varepsilon_{\perp} \tilde{\mathbf{E}} + \varepsilon_a (\tilde{\mathbf{E}} \cdot \mathbf{n}) \mathbf{n}) = 0 \quad \text{Conservation of charge}$$

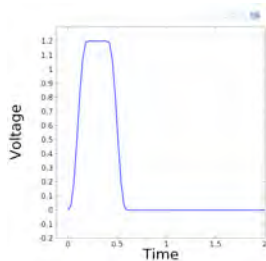
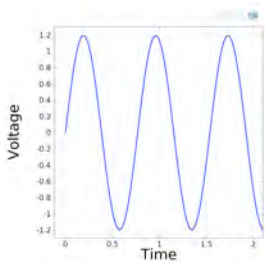
$$\tilde{\mathbf{E}} + \nabla v = 0 \quad \text{Electric Potential}$$

$$\Delta \tilde{p} - \tilde{p}_{,tt} = -\gamma \tilde{s}_{,tt} \quad \text{Pressure equation}$$

$$\text{where } s = \underbrace{\alpha_1 (\cos \theta_{\theta,y} - \sin \theta_{\theta,x})^2}_{\text{Splay coupling}} + \underbrace{\alpha_3 (\cos \theta_{\theta,x} + \sin \theta_{\theta,y})^2}_{\text{Bend coupling}}$$

Three different COMSOL physics are involved:

- (i) Electrostatics from the AC/DC Module - coupled with (iii) - for computing the electric potential
- (ii) Transient Pressure Acoustics from the Acoustic Module - coupled with (iii) - for computing the pressure
- (iii) Weak-form PDE from the Mathematics Module - coupled with (i) - for computing the nematic director field

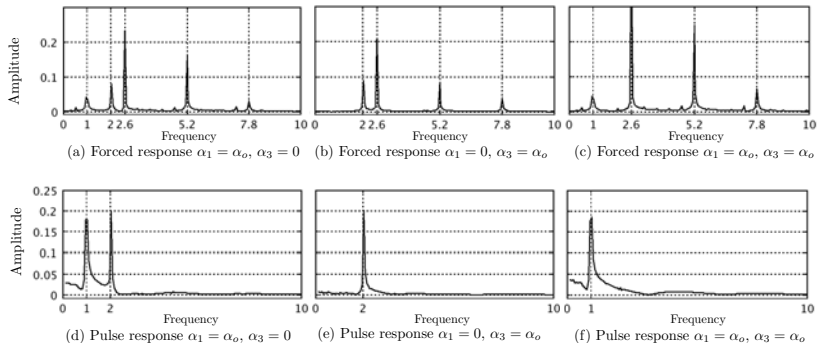


Two types of Voltage forcing terms are applied to the NLC sample

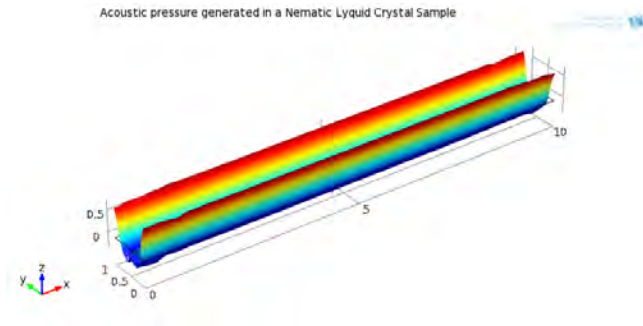
- (a) harmonic signal $V(t) = v_0 \sin(2\pi \tilde{f}_f \tilde{t})$
- (b) rectangular pulse of amplitude V_0 and length \tilde{t}_f ;

Where we assume $v_0 > v_F = 1$.

Spectra of the forced and transient response for different coupling constants



The results are in perfect agreement with those of Kim and Patel 1999



Snapshot of the sound pressure field at a given instant of the transient evolution

- the proposed model provides results in agreement with the experimental measures.
- the code obtained by coupling different physics provides good results for the non-linear system