POLITECNICO DI MILANO

Centre for Computational Structural and Materials Mechanics

A NUMERICAL APPROACH TO FIELD-INDUCED PHASE TRANSITIONS IN NEMATIC LIQUID CRYSTALS

Gaetano Napoli – Dipartimento di Matematica

Anna Pandolfi – Dipartimento di Ingegneria Strutturale

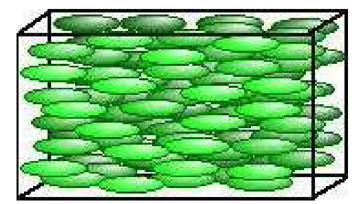
Seconda riunione Gruppo Materiali AIMETA
Genova, 29 Febbraio-1 Marzo 2008

Nematic Liquid Crystals

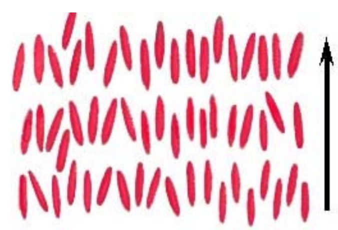
- Liquids characterized by the presence of anisotropic molecules, like rods or disks, may have orientational order in a liquid crystal state.
- The phases of a liquid crystal (LC) are defined by the amount of the order:
  - Nematic (NLC)
  - Smectic A, B or C (SLC)
  - Chiral or Cholesteric (CLC)

- NLC contains uniaxial achiral molecules aligned along an average direction called director **n**.
- The director can be aligned either through contact with a surface or by the application of an electric field.
- Conductivity and dielectric constants of NLC are different for electrics field applied normally or perpendicularly to the molecule axis.

Solid Liquid Crystals Liquid

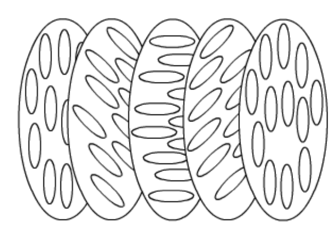


Nematic



Smectic A

Smectic C



Chiral - Cholesteric

Continuum Theory of the Director Field

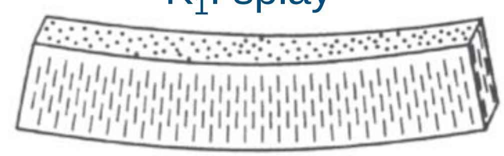
- For small changes of the director orientation from molecule to molecule, a continuum theory may be employed [Frank, 1958] where the director is assumed to be a function of the sole position:

$$\mathbf{n} = \mathbf{n}(\mathbf{x})$$

- The elastic free energy density of a NLC has the general form:

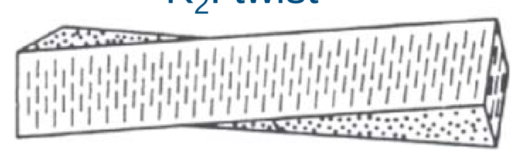
$$\psi_N = \frac{K_1}{2}(\mathrm{div}\,\mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n}\cdot\mathrm{curl}\mathbf{n})^2 + \frac{K_3}{2}|\mathbf{n}\times\mathrm{curl}\mathbf{n}|^2$$

K_1: splay



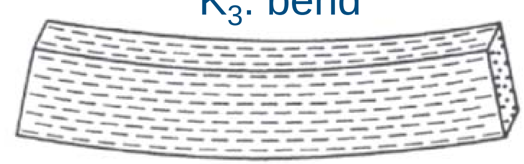
- K_1 , K_2 and K_3 are independent elastic constants describing the deformation modes of the NLC.
  From details of intermolecular interactions:

K_2: twist



$$K \approx \frac{\text{molecular interaction energy}}{\text{molecular separation}} = \frac{0.1\ eV}{1A} = 10^{-11}N$$

K_3: bend

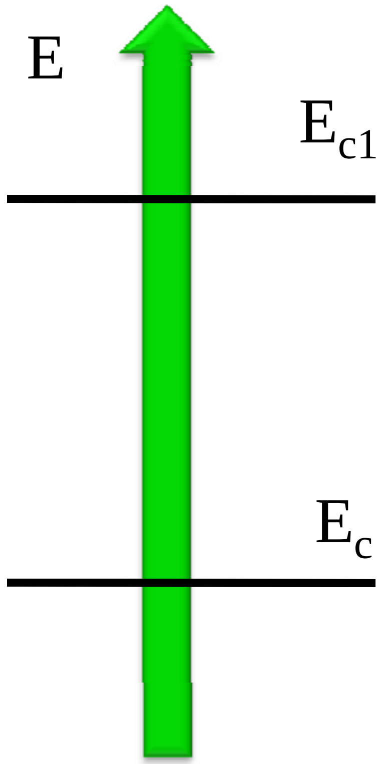


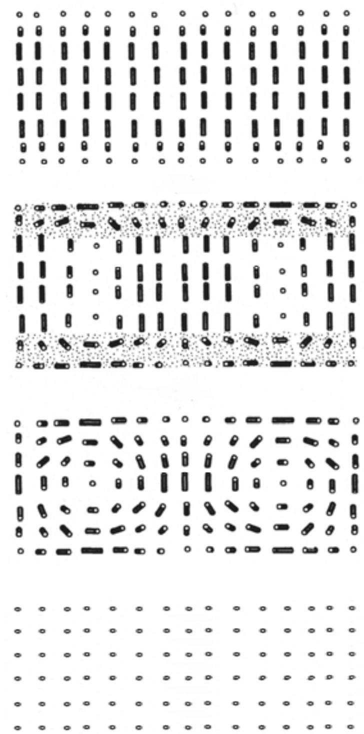
- Interaction energy of an electric field $\mathbf{E} = \mathrm{E}\ \mathbf{e}$ in a NLC (ε_a is the anisotropic dielectric constant):

$$\psi_{INT} = -\frac{1}{2}\varepsilon_a\,(\mathbf{E}\cdot\mathbf{n})^2$$

Configurational Distortions

- For a NLC between two flat glass plates (0.1 mm distance), changing the electric field intensity the orientation of the director may change.





High field $E > E_{c1}$: standard splay dominated distortion (Freederickzs transition).

Intermediate fields $E_c < E < E_{c1}$: for $K_1/K_2 > 3.3$, in proximity of the boundary splay is replaced by twist.

Fields immediately above $E_c <= E$: for a nematic with $K_1/K_2 > 3.3$, periodic twist dominated distortion.

Uniform field solution, with director aligned normally to the field and no distortion.

Analytical solutions of the phase transitions have been obtained only in asymptotic approximations (close to the bifurcation points, and in the case of uniform distortions for high fields). For intermediate and high fields, periodic distortions can be only obtained numerically.

Weak Formulation and Finite Element Approach

- NLC cell in a electric field, with strong planar anchoring boundary conditions at top and bottom surfaces. Minimize the total energy augmented with the unit length constraint, through Lagrangian multipliers λ. Get the Euler-Lagrange equations (with periodic boundary conditions):

$$\frac{\partial\psi}{\partial\mathbf{n}} - \mathrm{div}\left(\frac{\partial\psi}{\partial\nabla\mathbf{n}}\right) + 2\lambda\mathbf{n} = 0, \qquad \mathbf{n}^2 = 1$$

- Introducing test functions for both fields $\mathbf{n}$ and λ, write the weak form of equations:

$$\int_\Omega \left\{\left[\frac{\partial\psi}{\partial\mathbf{n}} + 2\lambda\mathbf{n}\right]\cdot\hat{\mathbf{n}} + \left(\frac{\partial\psi}{\partial\nabla\mathbf{n}}\right)\cdot\nabla\hat{\mathbf{n}} + (\mathbf{n}^2-1)\hat{\lambda}\right\} d\Omega + \int_\Gamma \hat{\mathbf{n}}\cdot\left(\frac{\partial\psi}{\partial\nabla\mathbf{n}}\right)\nu\, d\Gamma = 0,$$

- Upon discretization into 6-node 2D finite elements with nodal variables $\mathbf{u}_a$ (director) and μ_a (Lagrangian multiplier), obtain the algebraic nonlinear equation system (3th order polynomial):

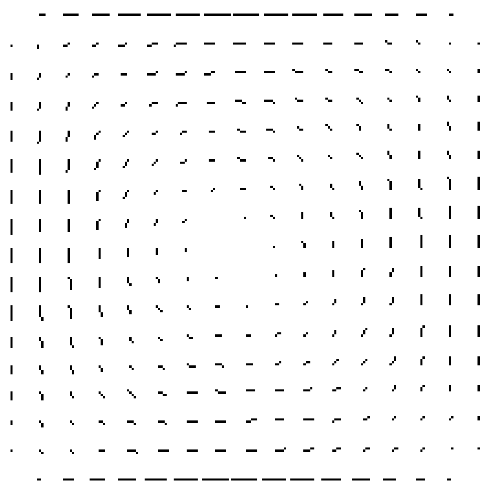
$$\mathbf{F}(\mathbf{D}) = \begin{bmatrix}\mathbf{H}_e(\mathbf{D})\\ G_e(\mathbf{D})\end{bmatrix} = \begin{bmatrix}\int_\Omega \mathbf{f}_e d\Omega + \int_\Gamma \mathbf{t}_e d\Gamma\\ \int_\Omega g_e d\Omega\end{bmatrix} = \mathbf{0}$$

- to be solved with a Newton-Raphson iterative procedure:

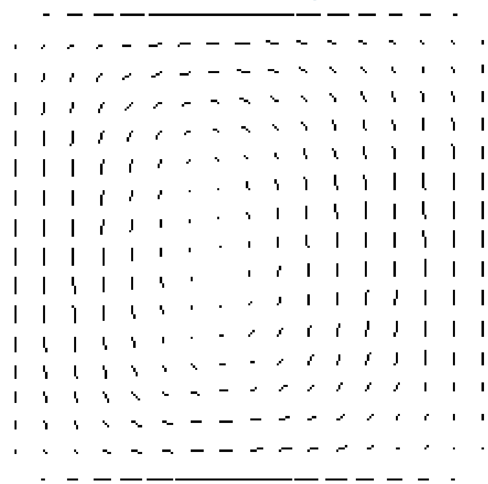
$$\mathbf{D}_{k+1} = \mathbf{D}_k - \left(\frac{\partial\mathbf{F}(\mathbf{D})}{\partial\mathbf{D}}\right)_k^{-1}\mathbf{F}_k(\mathbf{D})$$

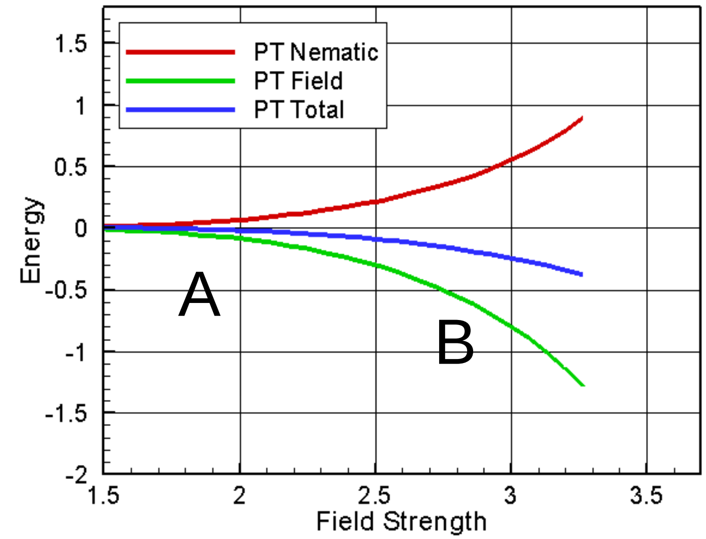
Numerical Solutions

A - Periodic Low Fields



B - Periodic High Fields

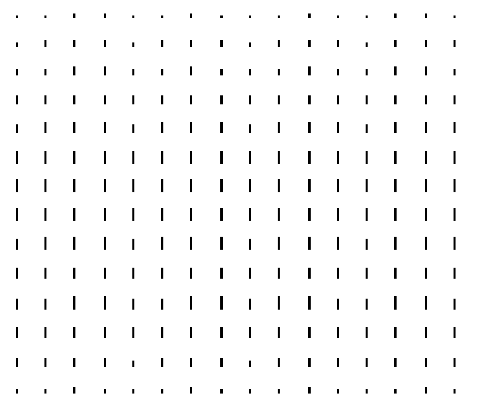


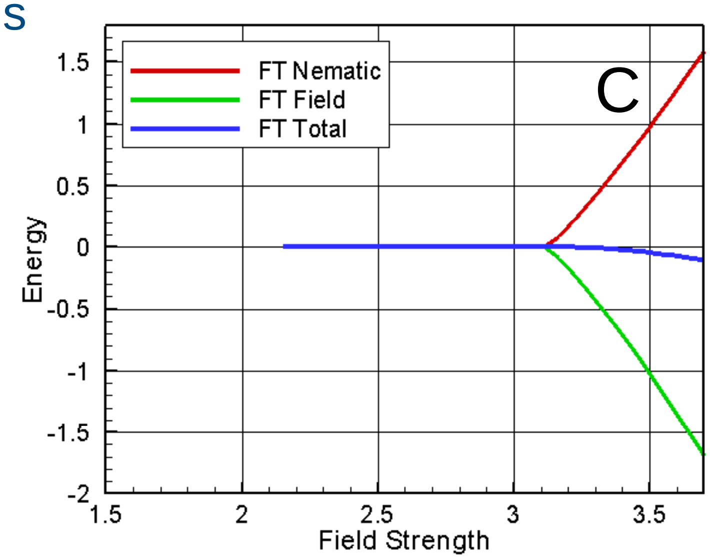


Periodic Transition

Standard Transition

C – Standard High Fields





References

- G. Napoli. Weak anchoring effects in electrically driven Freedericksz transitions. *Journal of Physics A: Mathematical and General, 39:11–31, 2006.*
- G. Srajer, F. Lonberg, and R. B. Meyer. Field-induced first-order phase transition and spinoidal point in nematic liquid crystals. *Physical Review Letters, 67(9):1102–1105, 1991.*
- F. Lonberg and R. B. Meyer. New ground state for the splay-Freedericksz transition in a polymeric nematic liquid crystal. *Physical Review Letters, 55(7):718–721, 1985.*
- V. Freedericksz and V. Zolina. Forces causing the orientation of an anosotropic liquid. *Transactions of the Faraday Society, 29:919, 1933*.