Nonlinear Elasticity and Liquid Crystals in Biological and Biomedical Applications

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Outline

Motivating examples of gel modeling and analysis

- Biomedical devices
- Gliding bacteria
- Cell motility in gel fiber matrix
- Gels and mixture theory
 - Constrained elasticity boundary value problems
 - Deformable porous media with polymer-fluid interaction
 - Free boundary problem of swelling
- Liquid crystals: remarks on fiber gels and polar particle flow
- Conclusions

Gels: polymeric networks, crosslinked or entangled, holding fluid [Tanaka, 81]

- Natural gels are found in animal tissue and plant bodies; cell membranes, cartilage,
- Synthetic gels are used in manufacturing devices such as actuators, valves, body implantable devices: artificial bone, skin, pacemakers, drug delivery units, ...

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Mathematical and modeling issues: Elasticity, diffusion, transport, dissipation, surface phenomena



Figure: Tibia bone prosthesis by Kasios

How much does it swell and how long does it take to settle down?

Bonding between different materials



- The lenght in figure A: 7.5 cm; the thikness of U-polymer (2 mm) versus S-polymer (5 mm). The length of the bent combination U/S (7.5cm). The length and thickness of polymer S in figure C (12 - 13 cm).
- S- Silicon, crosslinked, rubber-like polymer at room temperature; elastic module 10⁶ Pa; can absorbe hepthane (organic solvent) at the ratio of 300 to 400 percent of its volume.
- U- Polyurethane, linear polymer; elastic module 10⁸ Pa

Gels experience phase transitions between collapsed and shrunken phases driven by changes of temperature and pH, (also electric fields and light, in electrolite gels [Tanaka, 1978])



Bamboo pattern: regularly spaced cross-sectional planes, consisting of collapsed gels.



Bubble pattern: regions of bulges alternate with constrictions Assume gel as mixture of polymer and solvent.

$$\begin{split} \text{Mass} &: \; \frac{\partial \rho_i}{\partial t} + \text{div}(\rho_i \mathbf{v}_i) = \mathbf{0}, \\ \text{Linear momentum:} \; \rho_i \dot{\mathbf{v}}_i = \nabla \cdot \mathcal{T}_i + \mathbf{f}_i, \; \; i = 1,2 \end{split}$$

Assume gel as mixture of polymer and solvent.

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Volume fractions: $\phi_1 + \phi_2 = 1$

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- Cauchy stress tensor $\mathcal{T}_i = \mathcal{T}^r + \mathcal{T}^d$
- Reference configuration Ω_0 , $\mathbf{X} \in \Omega_0$
- Deformed configuration Ω_t , $\mathbf{x} \in \Omega_t$, t > 0
- polymer deformation map $\mathbf{x} = \mathbf{\Phi}(\mathbf{X}, t)$

▶ polymer deformation gradient $F = \nabla_{\mathbf{X}} \Phi$, det F > 0Component 1: polymer, Component 2: solvent, $\phi := \phi_1, \ \phi_2 = 1 - \phi_1$ $\phi = \phi(\mathbf{x}, t), \ \mathbf{v} = \mathbf{v}(\mathbf{x}, t)...$

Thermodynamics and constitutive assumptions

$$\mathcal{E} = \int_{\Omega_0} \{\mu(\phi_1)W(F) + \det F h(\phi_1, \phi_2)\} d\mathbf{X}$$

$$:= \int_{\Omega_0} \Psi(F, \phi_1) d\mathbf{X}$$

$$h(\phi_1, \phi_2) = a\phi_1 \log \phi_1 + b\phi_2 \log \phi_2 + \chi \phi_1 \phi_2$$

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h(φ

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$$\mathcal{T}_{1}^{r} = \phi_{1} \frac{\partial \Psi}{\partial F} F^{T} - (\phi_{1}p + \pi_{1})\mathcal{I}$$
$$\mathcal{T}_{2}^{r} = -(\phi_{2}p + \pi_{2})\mathcal{I}$$

•
$$\pi_i = \frac{\partial h(\phi_1, \phi_2)}{\partial \phi_i}$$
: osmotic pressure
• $\mathcal{T}_i = \mathcal{T}_i^r + \frac{\eta_i}{2} (\nabla \mathbf{v}_i + \nabla \mathbf{v}_i^T)$: Cauchy stress tensor

Incompressibility and Eulerian formulation of problem

Incompressible mixture $ho_i = \gamma \phi_i, \ \gamma = ext{constant} = 1$ (Minimise)

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 $\phi_1 \operatorname{det} F = \phi_0$

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$$\phi_{1} det F = \phi_{0}$$

$$\phi_{1} \frac{\partial \mathbf{v}_{1}}{\partial t} + \phi_{1}(\mathbf{v}_{1} \cdot \nabla)\mathbf{v}_{1} = \nabla \cdot \mathcal{T}_{1} - \beta(\phi)(\mathbf{v}_{1} - \mathbf{v}_{2}) + \phi_{1}\nabla p$$

$$\phi_{2} \frac{\partial \mathbf{v}_{2}}{\partial t} + \phi_{2}(\mathbf{v} \cdot \nabla)\mathbf{v}_{2} = \nabla \cdot \mathcal{T}_{2} + \beta(\phi)(\mathbf{v}_{1} - \mathbf{v}_{2}) - \phi_{1}\nabla p$$

$$\phi_{1} + \phi_{2} = 1$$

$$F_{t} + (\mathbf{v}_{1} \cdot \nabla)F = (\nabla \mathbf{v}_{1})F$$

diffusion coefficient $\mathcal{D} := \beta^{-1}(\phi_1)$ Unknowns: $\mathbf{v}_1, \mathbf{v}_2, \phi_1, \phi_2, p, F$





(2) Swollen and collapsed





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(3) Swollen and collapsed





(2) Swollen and collapsed



(3) Swollen and collapsed







Theorem

Let $\{\phi_i, \mathbf{v}_i, p\}$ be a smooth solution of the governing equations. Then it satisfies the following equation of balance of energy:

$$\begin{split} & \frac{d}{dt} \int_{\Omega(t)} [(\frac{\phi_1}{2} |\mathbf{v}_1|^2 + \frac{\phi_2}{2} |\mathbf{v}_2|^2) + \Psi] \, d\mathbf{x} \\ & - \int_{\partial\Omega(t)} (\mathbf{t}_1 \cdot \mathbf{v}_1 + \mathbf{t}_2 \cdot \mathbf{v}_2) \, dS \leq 0, \end{split}$$

Back

Boundary conditions

Let

$$\partial \Omega = \Gamma_1 \cup \Gamma_2, \ \Gamma_1 \cap \Gamma_2 = \emptyset$$

- Elasticity
 - 1. Displacement: $\mathbf{\Phi} = \mathbf{\Phi}_0$, on Γ_1
 - 2. Traction: $(\mathcal{T}_1 + \mathcal{T}_2)\boldsymbol{\nu} = \mathbf{t}_0$, on Γ_2
- Membrane permeability
 - 1. impermeable: $\frac{\partial \phi}{\partial \nu} = 0$ on $\partial \Omega$ (or part of it)
 - 2. fully permeable: $-\phi_2 p + \prod_2 (\phi_1, \phi_2) = P_0$,
 - P₀ pressure of surrounding solvent
 - Π_2 osmotic pressure of in-gel solvent
 - 3. semi-permeable: $P (p + \Pi_2(\mathbf{x}, t)) = \kappa(\mathbf{v}_2 \mathbf{v}_1) \cdot \nu$, $\kappa = \kappa(\phi) > 0$ permeability function

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- ► $\mathbf{V} := \phi_1 \mathbf{v}_1 + \phi_2 \mathbf{v}_2 = 0$, $\mathbf{U} := \mathbf{v}_1 \mathbf{v}_2 \neq 0$, neglect intertia terms & neglect Newtonian viscosity: diffusion model

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- ► Additional linearization of elasticity equations, neglect Newtonian viscosities, set φ = φ₀: stress-diffusion coupling model by Doi and Yamaue [2004]
- Neglect Newtonian viscosities: Start-up regimes; hyperbolic equations with weak damping

Equilibrium states: mixing regimes

$$\begin{split} \text{Minimize}\, \mathcal{E} &= \int_{\Omega_0} \{\phi_1 \, W(F) + \det F \, h(\phi_1, \phi_2)\} \, dX \\ \text{subject to } \phi_1 \det F &= \phi_0, \ 0 < \phi_0 < 1, \ u \in \mathcal{X}_{\Gamma} \end{split}$$

 $\mathcal{X}_{\Gamma} = \{ u : u \in W^{1,2\beta}, \ u = u_0 \text{ on } \Gamma \subset \partial \Omega_0, \ \text{det } F > 0, \ \text{a.e.} \}$

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$$W(F) := w(I_{\mathcal{C}}, II_{\mathcal{C}}, III_{\mathcal{C}}) \geq \alpha(I_{\mathcal{C}}^{\beta} + II_{\mathcal{C}}^{\gamma} + III_{\mathcal{C}}^{r}) + \gamma_{0},$$

- ► W polyconvex
- $\blacktriangleright \ \beta > \frac{3}{2}, \gamma \ge \frac{2\beta}{2\beta 1}, \ \alpha > 0, \ \gamma_0 \ge 0$
- g(s) := sh(¹/_s, 1 − ¹/_s), s ≥ 1, convex and monotonically decreasing

Existence of a minimizer follows from [Ball, 1977]

- ▶ $\beta > \frac{3}{2}$ gives a stronger restriction than $\beta = 1$ in general theorem: loss of elasticity occurs by increase of fluid volume fraction
- ► Condition on g follows from convexity of h(φ): 0 < χ < 1.5 (mixing regime)</p>
- Dependence of w on III_C is experimentally motivated by softenning of gel upon swelling
- Mixed displacement-traction boundary conditions hold in many applications

Equilibrium configurations: non-mixing regimes

Suppose that h is nonconvex with respect to φ; (χ > 1.5)
 Modify the energy to include |∇φ|²:

$$\int_{\Omega} \delta |\nabla \phi|^2 \, dx = \delta \int_{\Omega_0} \left| (\det(\nabla u))^{-\frac{1}{2}} \nabla_X \mathrm{A} dj \, (\nabla u) \right|^2$$

$$\begin{split} \text{Minimize}_{\{(u,\phi)\in X_{\infty}\}} \ \mathcal{E} \ &= \quad \int_{\Omega_0} \{\phi W(F) + \det F \ h(\phi, 1 - \phi)\} \ d\mathbf{X} \\ &+ \quad \int_{\Omega} \delta |\nabla \phi|^2 \ d\mathbf{x} \end{split}$$

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$$\begin{aligned} \mathcal{X}_{\infty} &= \{(u,\phi) : \phi \in \bar{\phi} + W^{1,2}, \ u \in \bar{u} + W^{1,\infty}_0, \ \phi \det F = \phi_0, \ \text{a.e.} \\ & 0 < \phi < 1, \ \|\nabla u\|_{L^{\infty}} < C < \infty\}, \\ & \bar{u} \in W^{1,\infty}, \ \bar{\phi} \in W^{1,2}, \ \text{prescribed} \end{aligned}$$

Theorem

Let $\Omega_0 \in \mathcal{R}^3$ be bounded, with Lipschitz boundary $\partial \Omega_0$. For any C > 0 there exits a minimizer of \mathcal{E} in \mathcal{X}_{∞} .

Remarks

- ► Prescription of Dirichlet boundary condition on φ = φ̄ corresponds to a fully permeable membrane boundary;
- ► Neumann boundary condition ∂φ/∂ν = 0 expresses impermeability; Robin condition in the case of semipermeable membrane

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- ► Neumann boundary condition ∂φ/∂ν = 0 expresses impermeability; Robin condition in the case of semipermeable membrane
- ► Taking 0 < δ << 1, solutions present boundary layer behavior near boundaries with prescribed displacement [MCC, Cockburn, 2008]
- Concentration of stresses occurs in boundary layers or in contact interfaces between two different materials
- This may cause bonding deterioration and breaking of the device

Sketch of the proof

- 1. $\|\nabla u\|_{L^{\infty}} < C$ implies det $\nabla u \leq 9C^3$
- 2. There is a minimizing sequence $\{\phi_h, u_h\} \in X_\infty$
- 3. Poincare inequality allows us to extract a subsequence, $u \rightharpoonup \bar{u}$ weak* in $W^{1,\infty}$
- 4. $0 < \phi_h < 1$, det $\nabla u_h > 1$ and $\phi_h > \frac{1}{9C^3}$
- 5. Obtain bound for $\int_{\Omega_0} |\nabla_X \phi_h|^2$
- 6. $u_h \rightharpoonup \bar{u}$ weak* in $W^{1,\infty}$ and $\phi_h \rightharpoonup \bar{\phi}$ weakly in $W^{1,2}$
- 7. Show that $\{\bar{\phi}, \bar{u}\} \in X_{\infty}$. Use the weak continuity of determinants
- 8. Proof of weak lower semicontinuity of last term in energy analogous to the case of liqud crystal elastomers [Calderer-Liu-Yan, 2006; 2008]

Remarks on Coupling of Elasticity and Cahn-Hilliard models

▶ Modify the equations of balance of mass by allowing diffusion:

$$\frac{\partial \rho_i}{\partial t} + (\mathbf{v}_i \cdot \nabla)\rho_i = -\frac{\delta \left(\Psi + |\nabla \phi_i|^2\right)}{\delta \phi_i}$$

•
$$\sum_{i=1,2} \frac{\delta\left(\Psi + |\nabla \phi_i|^2\right)}{\delta \phi_i} = 0$$
 holds

- Local balnce of mass constraint no longer valid
- Entropy inequality and subsequent dissipation are modified accordingly
- Approach appropriate to hydrogels with possibly large ionic effects

Gradient flow of coupled elasticity and Cahn-Hilliard models

H. Garcke [PhD. thesis, 2003] studied a generalized Ginzburg-Landau energy of the form:

$$egin{aligned} E(\mathbf{c},\mathbf{u}) &= \int_{\Omega} \{rac{1}{2} |
abla \mathbf{c}|^2 + \Phi(\mathbf{c}) + W(\mathbf{c},rac{1}{2}(
abla \mathbf{u} +
abla \mathbf{u}^T))\} \ &\sum_{i=1}^N c_i = 1 \end{aligned}$$

The governing system is:

$$\partial_t \mathbf{c} = L \Delta \mathbf{w}$$

$$\mathbf{w} = \mathbf{P}(-\nabla \cdot \nabla \mathbf{c} + \Phi_{\mathbf{c}}(\mathbf{c}) + W_{\mathbf{c}}(\mathbf{c}, \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\nabla \cdot S = 0$$

Proves existence of weak solutions also for the case that $\Phi(\mathbf{c})$ is logarithmic. Model related to the earlier Cahn-Larche, [1973]

Parameters

- ▶ *V_m* is the volume occupied by one monomer;
- ► N₁, N₂ denote the number of lattice sites occupied by the polymer and the solvent, respectively.
- N_x is the number of monomers between entanglement points;
- χ is the Flory interaction parameter;
- β is the polymer drag coefficient;
- μ is a scaling parameter related to the shear modulus.

$$\begin{array}{ccc} N_{x} & 20 \\ N_{1} & 1000 \\ N_{2} & 1 \\ V_{m} & .1nm^{3} \\ \chi & .5 \end{array}$$

Linear steady-state regime

$$\begin{split} \phi_0 \nabla \cdot \left((\lambda - \frac{2}{3}\mu) (\nabla \cdot \mathbf{u}) I + 2\mu E(\nabla \mathbf{u}) \right) \\ &= \nabla (p + \Pi_1 (\operatorname{div} \mathbf{u}) + \Pi_2 (\operatorname{div} \mathbf{u})) + \frac{\eta_1}{2} \operatorname{div} (\nabla \mathbf{v}_1 + \nabla \mathbf{v}_1^T) + \frac{\eta_2}{2} \operatorname{div} (\nabla \mathbf{v}_1 = u_t, \\ \nabla (a((1 - \phi_0) + \phi_0 \operatorname{div} \mathbf{u}) + (1 - \phi_0)p) \\ &= \beta (\operatorname{div} \mathbf{u}) (\mathbf{v}_1 - \mathbf{v}_2) + \frac{\eta_2}{2} \operatorname{div} (\nabla \mathbf{v}_2 + \nabla \mathbf{v}_2^T), \\ \nabla \cdot (\phi_0 \mathbf{v}_1 + (1 - \phi_0) \mathbf{v}_2) = 0 \end{split}$$

Coupling of steady state equations of compressible, dissipative elasticity with linear Stokes problem for fluids, with global incompressibility constraint. The second equation corresponds to Darcy's law with dissipation For prescribed displacement (or traction or mixed) boundary conditions for elasticity, membrane conditions for the fluid and initial conditions for \mathbf{u} , there exists a unique classical solution of the system. Moreover, the fields \mathbf{v}_1 and \mathbf{v}_2 decay to 0 as $t \to \infty$ [MCC, Chabaud, 2008]

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- System reduces to the model by Doi and Yamau [2004] upon setting tr ∇u = 0 and neglecting Newtonian viscosity
- Analogies with models analyzed by Douglas and Duran [1987] in oil recovery applications; the fluid phase may have two or more components
- Mathematical analogs found in geology in dealing with soil media and clays [Bennethum-Murad-Cushman, 2000]

Remarks on the nonlinear problem

$$\begin{split} \phi_1(\mathbf{v}_{1,t} + (\mathbf{v}_1 \cdot \nabla)\mathbf{v}_1) &= \operatorname{div} \, \mathcal{T}'(F, \phi_1) - \phi_1(\nabla p + \Pi_1(\phi_1)) \\ &+ \frac{\eta_1}{2} \operatorname{div} (\nabla \mathbf{v}_1 + \nabla \mathbf{v}_1^T) + \beta(\phi)(\mathbf{v}_1 - \mathbf{v}_2), \\ \phi_2(\mathbf{v}_{2,t} + (\mathbf{v}_2 \cdot \nabla)\mathbf{v}_2) &= -\phi_2 \nabla(p + \Pi_2) \\ &+ \frac{\eta_2}{2} \operatorname{div} (\nabla \mathbf{v}_2 + \nabla \mathbf{v}_2^T) + \beta(\phi)(\mathbf{v}_2 - \mathbf{v}_1), \\ \operatorname{div} (\phi_1 \mathbf{v}_1 + \phi_2 \mathbf{v}_2) &= 0, \\ F_t + (\mathbf{v}_1 \cdot \nabla) F &= (\nabla \mathbf{v}_1) F, \\ \mathcal{T}' &= \frac{\partial \Psi(\phi_1, F)}{\partial F} \end{split}$$

- Coupling of nonlinear elasticity with Navier-Stokes with gel incompressibility constraint
- Difficulty with chain rule equation relating Lagrangian and Eulerian variables
- ► Local existence of weak solutions for small strains [MCC].

Oldroyd-B model

$$\mathbf{v}_t + (\mathbf{v} \cdot \nabla)\mathbf{v} + \nabla p = \eta \nabla \mathbf{v} + \operatorname{div} (F^T F)$$
$$F_t + (\mathbf{v} \cdot \nabla)F = (\nabla \mathbf{v})F$$
$$\operatorname{div} \mathbf{v} = 0$$

- Global existence of classical soluions near equilibrium [Lin, Liu, Zhang, 2006]
- Global existence of weak solution in 2-d [Lin, June 2008]
- Global existence of weak solutions with modified equation $F_t + (\mathbf{v} \cdot \nabla)F = \Omega(\nabla \mathbf{v})F, \Omega$ skew [P.L.Lions, Masmoudi]
- Global existence of appropriately small weak solutions with modified equation $F_t + (\mathbf{v} \cdot \nabla)F = (\nabla \mathbf{v})F \gamma F$ [Guilloupe, Saut]

Example: 1-D free boundary problem of swelling

- Neglect Newtonian dissipation and assume Neo-Hokean elasticity
- Assume perfect boundary permeability
- $u := v_1 v_2$

$$\begin{split} \phi_t &+ [\phi(1-\phi)u]_x = 0, \\ u_t &+ [\frac{1}{2}(1-2\phi) - G(\phi)]_x = -\frac{\beta u}{\phi(1-\phi)}, \\ \phi(x,t) &= \phi^*, \text{ at } x = \pm S(t). \\ S'(t) &= [1-\phi(S(t),t)]u(S(t),t), \ S(0) = L, \\ \phi(x,0) &= \phi^0, \ u(x,0) = u^0, \text{ for } -L < x < L \end{split}$$

The system is strictly hyperbolic if

$$G'(\phi)+u^2<0$$

- G'(φ) < 0 for polymers used in devices
- For polyssacharides, $G'(\phi) \ge 0$, $\phi \in (0, a) \subset (0, 1)$; the critical value $G'(\phi_c) = 0$ may suggest onset of de-swelling

How Myxobacteria Glide?



Electron micrograph of an isolated cell of M. santhus DK1622 showing one of the cells poles; nozzles are ring like structures seen at pole

C.Wolgemuth, E.Holczyk, D.Kaiser and G.Oster [2002]



Figure: Electron micrograph of nozzles



Figure: Schematic illustration of nozzle arrangement in cell

Local wellposedness

$$u_t + F(u)_x + G(u) = 0,$$
 (1)
 $t = 0: u = u_0$ (2)

Local wellposedness

$$\mathbf{u}_t + \mathbf{F}(\mathbf{u})_x + \mathbf{G}(\mathbf{u}) = 0, \qquad (1)$$

$$t = 0: \ \mathbf{u} = \mathbf{u}_0 \qquad (2)$$

$$\mathbf{u} := [\phi, \ u]^{T}, \\ \mathbf{F} := [\phi(1 - \phi)u, \ \frac{1}{2}u^{2}(1 - 2\phi) - G(\phi)]^{T}, \\ \mathbf{G} := [0, \frac{\beta u}{\phi(1 - \phi)}]^{T}$$

- The system admits an entropy-entropy flux pair $(\eta(\mathbf{u}), \mathbf{q}(\mathbf{u}))$, with $\eta(\mathbf{u})$ convex [MCC, Zhang, 2007]
- Local well posedness of the Cauchy problem

The following properties hold:

- The equilibrium solution $\mathbf{u}_e := (\phi^*, \mathbf{0})$ is L^1 -stable
- ► The function **G** is weakly dissipative

Consider initial data $\mathbf{u}_0 \in B_r(\mathbf{u}_e)$, $\|\mathbf{u}_e - \mathbf{u}_0\|$, $\mathrm{TV}_{(-\infty,\infty)}\mathbf{u}_0 < \infty$ small enough.

Then there exists an admissible global BV solution to the Cauchy problem

Perform chage of variables of gas dynamics:

$$y := \int_{\mathcal{S}(t)}^{x} \phi(z,t) dz, \ \tau = t$$

Then

$$(-S(t),S(t))\longrightarrow (0,1)$$

For sufficiently small initial data, there exists a unique global C^1 -solution of the system [Chen, MCC, 2008]

Mesenchymal motion describes cellular movement in tissues formed by fiber networks

- Interacting system of polymer, solvent and cells
- Fibers are elastic and highly orientable, forming uniaxial liquid crystal network [Barocas, Tranquillo, 2004]
- Cells cause fiber degradation upon perpendicular impact
- They flow as polar liquid crystals [Painter, 2008; Bischofs, Schwarz, 2008]

Uniaxial order tensor: $Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I)$ How to measure Q?

Dielectric tensor in small molecule nematic liquid crystals,

$$\mathcal{D} = arepsilon_{\perp} I + arepsilon_{a} \mathbf{n} \otimes \mathbf{n}, \;\; arepsilon_{a} = arepsilon_{\parallel} - arepsilon_{\perp}$$

- Diffusion tensor in fibers; the counterparts of ε parameters represent the anisotropic diffusion coefficients.
- Fiber matrix presents liquid crystal point defects: Are they nucleation sites of tumors?

HAPPY BIRTHDAY !!!!!!!!