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Topics in the Mechanics of Soft and Biological Matter

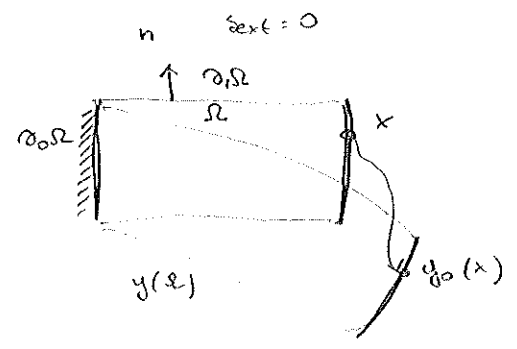
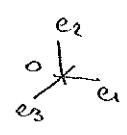
Contents

1. Classical rubber elasticity (review with a hands-on perspective)
2. Liquid Crystal Elastomers (mostly modeling)
3. Relaxation and quasi-convex envelopes (mostly analysis)
for LCE energies
4. Mobility of small scales and
biological self-propulsion

1. Nonlinear Elastostatics

Typical BVP for hyperelastic materials

$$\begin{aligned} \text{Div } S + b_0 &= 0 & \text{in } \Omega \\ S n &= s_{\text{ext}} & \text{on } \partial_1 \Omega \\ y &= y_0 & \text{on } \partial_0 \Omega \end{aligned}$$



where

$y: \Omega \rightarrow \mathbb{R}^d$, def. map (globally inv.)

$F = \nabla y$ def. quad, $\det F > 0$

$$S(x) = \partial_F W(F(x)) = \partial_F W(\nabla y(x))$$

$$S_{ij} = \frac{\partial}{\partial F_{ij}} W$$

W energy density (a free-energy)

S 1st Piola-Kirchhoff stress.

$$u(x) = y(x) - x \quad \text{displacement at } x$$

Unknown: $y: \Omega \rightarrow \mathbb{R}^d$, def. map.

- Data:
- b_0, s_{ext} given functions of x alone
forces p.u. ref. volume/area at each x
 - Dead loads: must be indep. of y -flow??
 - y_0 prescribed function on $\partial_0 \Omega$

The data involve "traction" and "displacement" BC's. Once y is known, can determine def. field $F(x) = \nabla y(x)$ and stress distribution $S(x) = \partial_F W(\nabla y(x))$.

Solutions of BVP above are stationary points for the energy-functional

$$\begin{aligned} I(y) &= \underbrace{\int_{\Omega} W(\nabla y(x)) dx}_{\text{stored elastic energy}} - \underbrace{\int_{\Omega} b_0(x) \cdot y(x) dx - \int_{\partial_1 \Omega} s_{\text{ext}} \cdot y(x) dx}_{\text{work done by ext. forces}} \\ &= - \int_{\Omega} b_0(x) \cdot (y(x) - x) dx = - \int_{\Omega} b_0 \cdot y + \text{const.} \end{aligned}$$

subject to $y = y_0$ on $\partial_0 \Omega$.

Take $\delta y = \epsilon u$, $u = 0$ on $\partial\Omega$ and consider

$$I(y + \epsilon u) = \int_{\Omega} W(\nabla y + \epsilon \nabla u) - \int_{\Omega} b_0 \cdot (y + \epsilon u) - \int_{\partial, \Omega} s_{ext} \cdot (y + \epsilon u)$$

I stationary at y implies

$$\frac{d}{d\epsilon} I(y + \epsilon u) \Big|_{\epsilon=0} = \int_{\Omega} \underbrace{\sigma_F W(\nabla y)}_{S(\nabla y)} \cdot \nabla u - \int_{\Omega} b_0 \cdot u - \int_{\partial, \Omega} s_{ext} \cdot u = 0 \quad \forall u$$

[virtual work done by int. stresses = virtual work done by ext. forces + virt. work of perturbation $y(\epsilon)$]

Since

$$\text{Div}(S^T u) = \text{Div} S \cdot u + S \cdot \nabla u$$

$$[(s_{ji} u_j)]_{,i} = s_{j,i} u_j + s_{ji} u_{j,i}$$

we have

$$0 = \int_{\Omega} \text{Div}(S^T u) - \int_{\Omega} (\text{Div} S + b_0) \cdot u - \int_{\partial, \Omega} s_{ext} \cdot u$$

$$= \int_{\partial, \Omega} (s_{in} - s_{ext}) \cdot u - \int_{\Omega} (\text{Div} S + b_0) \cdot u \quad \forall u$$

Take $u \in C_0^\infty(\Omega)$ to get $\text{Div} S + b_0 = 0$, then take u vanishing on $\partial\Omega$ but arbitrary on ∂, Ω to get $s_{in} = s_{ext}$ on ∂, Ω . Thus, crit. pts of I are solutions of the equilibrium pbs.

For W, I strictly convex, the only crit. pt is the minimum of I . Conversely, it is unrealistic, but we'll keep minimum energy because minimum free energy is the correct physical principle for equilibrium in isothermal conditions.

Incompressible case

Under normal loading conditions, rubber deforms experiencing negligible volume changes (shear modulus \ll bulk modulus)

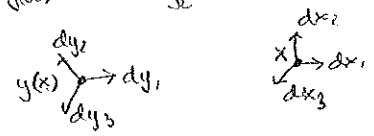
Volume preserving def's. $\det \nabla y(x) \equiv 1$.

Re: formula for change of var's in volume int. involves jacobian determinant of the map giving transf. of coordinates

This places a constraint on admissible def's.

Deal with it using Lagrange multiplier technique

$$\int_{y(x)} f(y) dy = \int_{x} f(y(x)) \det \nabla y(x) dx$$



$$y(x + dx_i) \approx y(x) + F dx_i$$

$$\frac{dy_j}{dx_i} = \frac{dV_j}{dV_i} = \frac{F_{dx_1} \times F_{dx_2} \cdot F_{dx_3}}{dx_1 \times dx_2 \cdot dx_3} = \det F$$

$$\tilde{I}(y, \pi) = J(y) - \int_{\Omega} \pi(x) (\det \nabla y(x) - 1) dx$$

$$\tilde{I}(y + \epsilon u, \pi + \epsilon \delta \pi) = \dots - \int_{\Omega} (\pi + \epsilon \delta \pi) (\det(\nabla y + \epsilon \nabla u) - 1)$$

$$\left. \frac{d}{d\epsilon} \tilde{I} \right|_{\epsilon=0} = \dots - \int_{\Omega} \underbrace{\pi \partial_F \det(\nabla y)}_{\text{cof } \nabla y} \cdot \nabla u - \int_{\Omega} \delta \pi (\det \nabla y - 1) = 0 \quad \forall u, \delta \pi$$

Re: $\text{cof } F$: matrix of id. minors / cofactors.

For F invertible $\text{cof } F = (\det F) F^{-T}$ because $F^{-1} = \frac{1}{\det F} (\text{cof } F)^T$

$$f(F+U) = f(F) + Df(F)[U] + \delta(U)$$

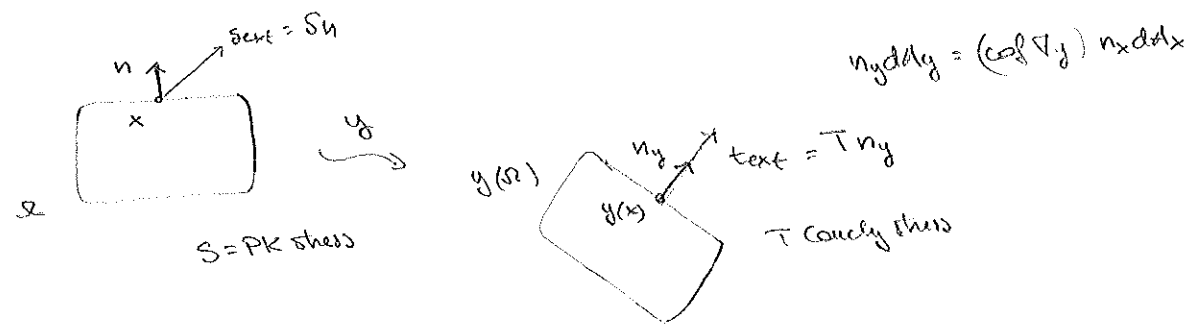
$$\begin{aligned} \det(F+U) &= \det F + U \cdot \text{cof } F + \text{cof } U \cdot F + \det U \\ &= \det F + \underbrace{(\text{cof } F) \cdot U}_{\text{tr}_F \det(F)} + \delta(U) \end{aligned}$$

We obtain

$$\int_{\Omega} \underbrace{(\partial_F W(\nabla y) - \pi \text{cof } \nabla y)}_{S(\nabla y, \pi)} \cdot \nabla u - \int_{\Omega} b \cdot u - \int_{\partial \Omega} \delta \pi \cdot u - \int_{\Omega} \delta \pi (\det \nabla y - 1) = 0 \quad \forall u, \delta \pi$$

Everything as before, except that now the stress is not entirely determined by the deformations, but includes a "reactive part" (reaction to incompressibility constraint). The scalar π , called pressure, is a further unknown of the BVP.

Remark π is the same pressure we use to include as $-\pi I$ in the real world of Cauchy stresses. Formula for change of variables in surface integrals.



$$\int_{\partial y(\Omega)} T(y) n_y dA_y = \int_{\partial \Omega} \underbrace{T(y(x)) \text{cof } \nabla y(x)}_{S} n_x dA_x = \int_{\partial \Omega} S n_x dA_x$$

$$S = T \text{cof } F = (\det F) T F^{-T}$$

If $T = -\pi I$, then $\text{tr} T = -\pi n_y$
 $\text{ext} = S n_x = -\pi \text{cof } \nabla y(x) n_x$

[same direction of $\text{tr} T$ and ext (!)]

Thm of power expended (conservation of energy).

Given a one-parameter of equilibrium states $\tau \mapsto y(x, \tau)$ [e.g., solutions of BVP under a one-par. family of displacement/traction BCs], then

$$\frac{d}{dt} \int_{\Omega} W(\nabla y(x, \tau)) dx = \int_{\Sigma} b_0 \cdot \underbrace{\frac{\partial}{\partial \tau} y}_{\dot{y}} + \int_{\partial \Omega} S n \cdot \underbrace{\frac{\partial}{\partial \tau} y}_{\dot{y}}$$

$\tau = \text{time}$

Proof: Exercise (test eqn's against \dot{y} + integrate by parts) //

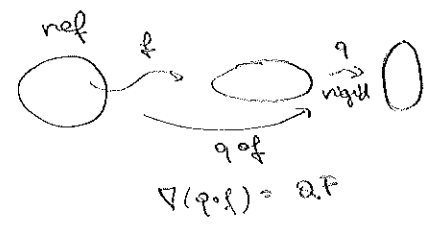
Remarks, Physical meaning: in the absence of dissipation, the rate at which we store energy

- is exactly the rate at which external work is performed on the system.
- It holds for both compressible and incompressible cores
- Extremely useful in the analysis of BVPs reproducing standard mech tests (study of discontinuity stress-strain response of engineering materials).

Constitutive Theory

a) Frame-indifference (FI): $\forall F$

$W(QF) = W(F) \quad \forall Q \in \text{Rot}$



A basic requirement for physical plausibility (and with a given of self: linear elasticity is not FI).

A consequence: Usual w.r.t polar decomposition of F

$Q = R^T$

Re: $F = RU, \quad U = (F^T F)^{1/2} \in \text{PSym} \quad (\text{polar decoup.})$

$W(F) = W(QF) = W(R^T U) = W(U)$

Define

$\tilde{W}(C) = \tilde{W}(F^T F) = W(C^{1/2})$

get

$W(F) = \tilde{W}(F^T F)$

[Frame indifference of W also leads automatically to symmetry of Cauchy stress, which guarantees that also balance of torques is satisfied]

Re: Polar decomposition

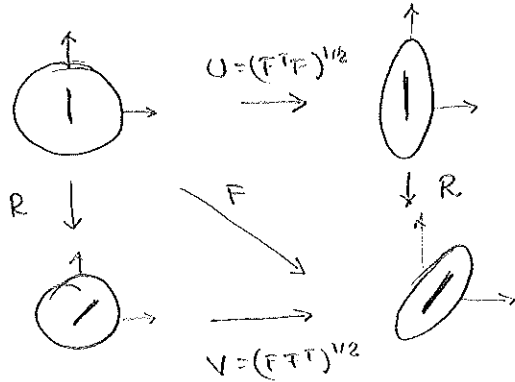
F with $\det F > 0$, then $\exists!$ $R \in \text{Rot}$, $U, V \in \text{PSym}$ s.t.

$$F = RU = VR$$

Since $V = RUR^T$, V has same values of U and vectors rotated by R

$$(\omega_i(V), e_i(V)) = (\omega_i(U), R e_i(U))$$

Schematic diagram



$$e \mapsto Fe$$

$$|Fe|^2 = Fe \cdot Fe = F^T F e \cdot e$$

$$\max_{|e|=1} \left[\frac{|Fe|^2}{|e|^2} \right]^{1/2} = \max_{|e|=1} \left[(F^T F) e \cdot e \right]^{1/2} = \omega_{\max}^{1/2}(F^T F) = \omega_{\max}(U)$$

$\omega_{\max}(U)$, $e_{\max}(U)$ give direction of material fiber which is maximally stretched by F (reference orientation)

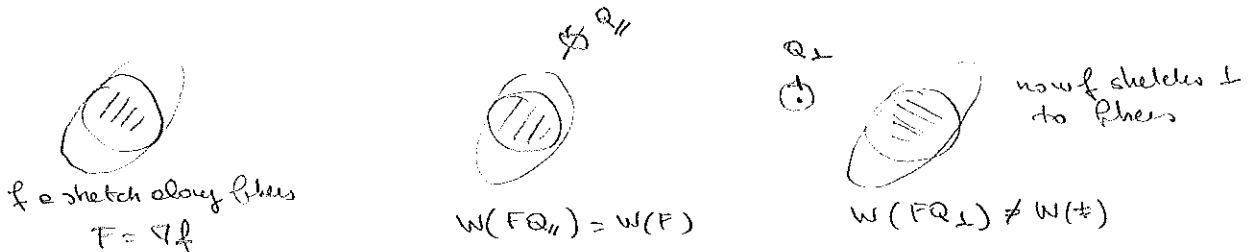
$\omega_{\max}(V)$, $e_{\max}(V) = R e_{\max}(U)$ give the current orientation of the direction which is maximally stretched by F . (current orientation = after deformation).

b) Material Symmetry. $Q \in$ symmetry group of the material \Leftrightarrow only $\forall F$,

$$W(FQ) = W(F)$$

[rotations of the ref. configurations that are not detectable by energy density, hence by mech. testing]

E.g. for a material with oblique fibers.



Isotropic materials are those with NO special directions at all, i.e. their symmetry groups = Rot

$$\forall F, \quad W(FQ) = W(F) \quad \forall Q \in \text{Rot} \quad (\text{Iso}).$$

For isotropic, FI materials, the energy density can only depend on the principal stretches (sq. roots of values of $B = FF^T$ or $C = F^T F$) or, equivalently, on the invariants of B or C .

$$\left. \begin{aligned} W(QF) &= W(F) \\ W(FQ) &= W(F) \end{aligned} \right\} \forall Q \in \text{Rot} \Rightarrow W(F) = \left\{ \begin{aligned} \tilde{W}(FF) \\ \tilde{W}(Q^T F^T F Q) \end{aligned} \right\} \forall Q \in \text{Rot} = \tilde{W} \left(\begin{bmatrix} \lambda_1^2(F) & 0 & 0 \\ 0 & \lambda_2^2(F) & 0 \\ 0 & 0 & \lambda_3^2(F) \end{bmatrix} \right)$$

use Q that diagonalizes $F^T F$

or

$$W(F) = \tilde{f}(\lambda_1(F), \lambda_2(F), \lambda_3(F)), \quad \text{where } \lambda_i(F) = \omega_i^{1/2}(C) = \omega_i^{1/2}(B)$$

principal stretches, or singular values of F values of C and B

Rubber Elasticity

Neo-Hookean model

$$W(F) = \frac{1}{2} \mu [\text{tr}(FF^T) - 3], \quad \det F = 1$$

$\mu > 0$ shear modulus

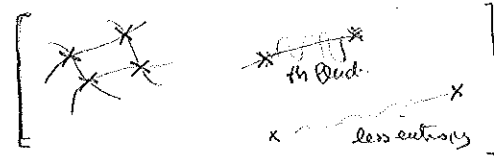
Equivalent expressions: $\left\{ \begin{aligned} &\frac{1}{2} \mu [F \cdot F - 3], \\ &\frac{1}{2} \mu [I_1 - 3], \quad \frac{1}{2} \mu [\text{tr} B - 3], \quad \frac{1}{2} \mu [\text{tr} C - 3], \quad \frac{1}{2} \mu [\lambda_1^2(F) + \lambda_2^2(F) + \lambda_3^2(F) - 3] \end{aligned} \right.$

$$W(F) = \begin{cases} \frac{1}{2} \mu [\text{tr}(FF^T) - 3] & \text{if } \det F = 1 \\ +\infty & \text{else} \end{cases}$$

Remarks

- W depends only on principal stretches: it's ISO and FI
- This is a hard conceptual model, like perfect gas law $p = nRT/V$, not a tool for determining times.
- It can be derived from stat mech: it's entropic elasticity of phantom gaussian chains.
- Useful, because it leads to $\mu = n k_B T$ (the material stiffens with temperature).

Restoring force opposing stretching is due to decrease in entropy (lower number of microscopic realizations for a stretched state).



$$W(F) \geq 0 \quad \forall F, \quad W(F) = 0 \Rightarrow F \in \text{Rot}$$

Nothing to prove if $\det F \neq 1$. If $\det F = 1$, then (\neq between arithmetic and geometric mean) \Rightarrow strict concavity of the logarithm

$$\underbrace{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}_{\text{tr} B} \geq 3 \underbrace{(\lambda_1^2 \lambda_2^2 \lambda_3^2)^{1/3}}_{\det F^2 = \det B = 1} = 3$$

= only if $\lambda_1^2 = \lambda_2^2 = \lambda_3^2$ which, together with $\lambda_1 \lambda_2 \lambda_3 = 1 \Rightarrow \lambda_i = 1, i=1,2,3$

This implies $B = I$ and $F = B^{1/2} R \in \text{Rot}$.

Mechanical tests Assume specimen behaves as neo-hookean. Simulate outcome of mech exp's. 1/7
2/2

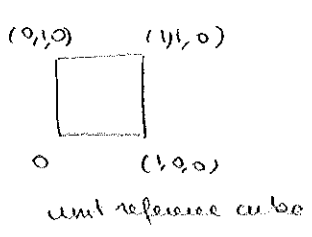
Small specimens, neglect gravity ($b_0 = 0$).

Enforce affine deformations (easier interpretation: def. can be estimated from boundary measurements)

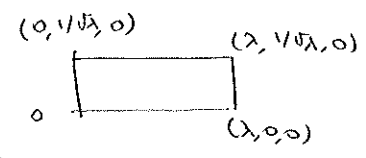
$F = \text{const.} \Rightarrow S = \partial_F W(F) = \text{const.} \Rightarrow \text{Div } S + b_0 = 0$ locally satisfied.

Equal pts. reduces to checking consistency of F with different / hooking BCs.

e) Uniaxial extension



extend along e_1 by λ
along \perp directions unaccounted



by symmetry $F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}$

$y(x) - 0 = F \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$

Q: How to realize this? If pull on vertical edges



On lateral surfaces, $S_n = S_{nt} = 0$

[Re: $S_{ij} = S_{ej} \cdot e_i$]

On $x_1 = 0$, $y_1 = \lambda x_1 = 0 \Rightarrow S_{e_1} \cdot e_1 \neq 0$

y_2, y_3 free $\Rightarrow S_{e_1} \cdot \begin{bmatrix} e_2 \\ e_3 \end{bmatrix} = 0$

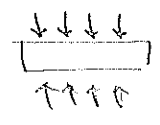
[If const pressure this]

On $x_1 = 1$, $y_1 = \lambda x_1 = \lambda \Rightarrow S_{e_1} \cdot e_1 \neq 0$

y_2, y_3 free $\Rightarrow S_{e_1} \cdot \begin{bmatrix} e_2 \\ e_3 \end{bmatrix} = 0$

region of a fluid def. but do local moments of F , cannot only rely on boundary measurements

Alternatively, could be pulling on lateral faces, leaving vertical ones free



Analysis of the experiment, assume

$F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}$, $\text{cof } F = \frac{dF}{dF} F^{-T} = \begin{bmatrix} 1/\lambda & 0 & 0 \\ 0 & \sqrt{\lambda} & 0 \\ 0 & 0 & \sqrt{\lambda} \end{bmatrix}$

$W(F) = \frac{1}{2} \mu (F \cdot F - 3)$

$S = \partial_F W(F) - \pi \text{cof } F = \mu F - \pi \text{cof } F$

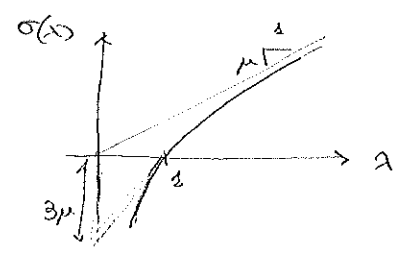
[$W(F+U) = (F+U) \cdot (F+U) = F \cdot F + F \cdot U + U \cdot F + U \cdot U = W(F) + 2F \cdot U + O(U)$]

$= \mu \begin{bmatrix} \lambda & & \\ & 1/\sqrt{\lambda} & \\ & & 1/\sqrt{\lambda} \end{bmatrix} - \pi \begin{bmatrix} 1/\lambda & & \\ & \sqrt{\lambda} & \\ & & \sqrt{\lambda} \end{bmatrix}$

$$S_{22} = S_{33} = 0 \Rightarrow \mu \frac{1}{\sqrt{\lambda}} - \pi \sqrt{\lambda} = 0 \Rightarrow \pi = \frac{\mu}{\lambda}$$

$$S_{11} = \mu \lambda - \pi \frac{1}{\lambda} = \mu \lambda - \mu \frac{1}{\lambda^2} = \mu \left(\lambda - \frac{1}{\lambda^2} \right) = \sigma(\lambda)$$

$$\left. \frac{d}{d\lambda} \sigma(\lambda) \right|_{\lambda=1} = \mu \left(1 + \frac{2}{\lambda^3} \right) \Big|_{\lambda=1} = 3\mu$$



Can get $\sigma(\lambda)$ from the of power expended

$$\int_{y_1=0}^{y_2=\lambda} \sigma(\lambda) = S_{11}(\lambda) \quad \frac{d}{d\lambda} \int_{\Omega} W(F(\lambda)) = 1 \times 1 \times 1 \frac{d}{d\lambda} \left(\frac{1}{2} \mu \left(\lambda^2 + \frac{2}{\lambda} \right) \right) = \mu \left(\lambda - \frac{1}{\lambda^2} \right)$$

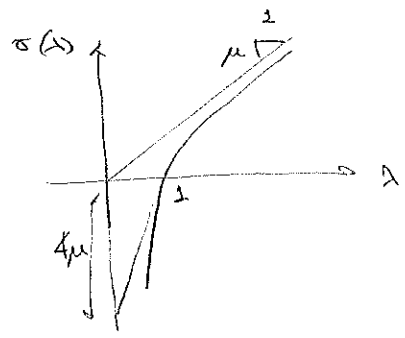
$$\int_{\partial \Omega} S(F(\lambda)) n \cdot \frac{d}{d\lambda} y = 1 \times 1 \cdot S_{11}(\lambda) \cdot 1$$

Remark: Not realistic, Ogden-type energies for stiffening at high stretches.

b) Plane stress extensor, (or pure shear)

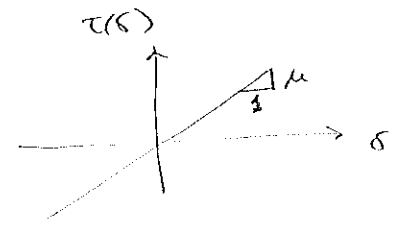
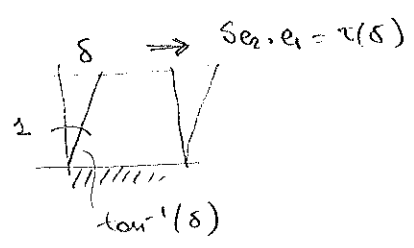
$$F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\lambda & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{no deformation in z-direction.}$$

Arms $\Rightarrow \sigma(\lambda)$ get



c) Simple shear

$$F = \begin{bmatrix} 1 & \delta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

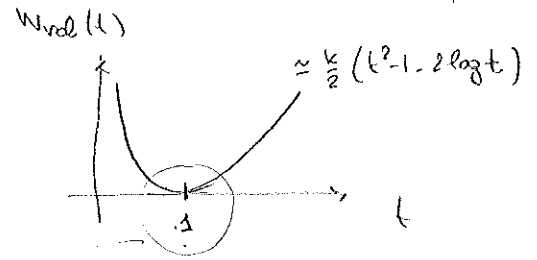


Compressible case

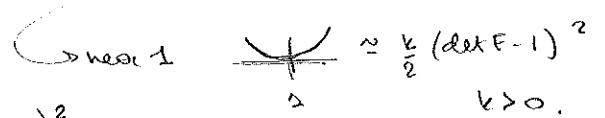
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$$W = W_{dev}(F), \quad \det F = 1$$

$$W_{coup}(F) = W_{dev}((\det F)^{-1/3} F) + W_{vol}(\det F)$$



E.g., for Neo-Hookean near $B = I$



$$W_{coup}(B) = \frac{1}{2} \mu \left((\det B)^{-1/3} \text{tr} B - 3 \right) + \frac{k}{2} \left(\det(B^{1/2}) - 1 \right)^2$$

Small strain theory (geometrically linear theory)

Assume $B = I + 2E$, E small

$$\begin{aligned} W_{coup}(B) &= \frac{1}{2} \mu \left((\det B)^{-1/3} \text{tr} B - 3 \right) + \frac{k}{2} \left(\det(B^{1/2}) - 1 \right)^2 \\ &= \frac{1}{2} \mu \left((\det(I+2E))^{-1/3} \text{tr}(I+2E) - 3 \right) + \frac{k}{2} \left(\det(I+2E)^{1/2} - 1 \right)^2 \\ &\quad \downarrow \qquad \qquad \qquad \downarrow \\ &= \mu |E_d|^2 + \frac{k}{2} (\text{tr} E)^2 \end{aligned}$$

deviatoric part of E .

where $E_d = E - \frac{1}{3}(\text{tr} E)I$ and we have used

$$\det(I+H) = 1 + \text{tr} H + \text{tr} \text{cof} H + \det H$$

$$(I+2E)^{1/2} = I + E + \dots$$

Taylor expansions of various functions.

Since $F = I + \nabla u$

$$B = F F^T = (I + \nabla u)(I + \nabla u^T) = I + 2 \text{sym} \nabla u + \nabla u \nabla u^T$$

we identify E in $B = I + 2E$ with $\text{sym} \nabla u$ and obtain the variational formulation of isotropic linear elasticity

$$I(u) = \int_{\Omega} \mu |\text{sym} \nabla u|_d^2 + \frac{k}{2} (\text{div} u)^2 - \int_{\Omega} b \cdot u - \int_{\partial, n} \text{ext} \cdot u + BCs$$

where $u(x) = y(x) - x$ is the displacement
 $\mu > 0$ shear modulus
 $k > 0$ bulk modulus.

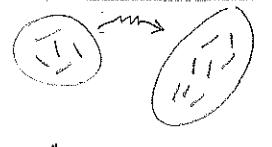
[Rigorous proof by
 Ciarra - convergence,
 Agostiniani et al, 2011]

2. Nematic Elastomers

NEs w/out current non stretch $\epsilon_{non}(V) // n$, current nematic director.

$$\omega_{non}(V) = (Q^{1/3})^2$$

$F = I$ $F = L^{1/2}(n)$



$\uparrow n, |n|=1$

$\uparrow N = non$ ($\pm n$ symmetry)

[de Gennes order tensor, Forminvarial sparsity case
 $Q = s(n \otimes n - \frac{1}{3} I)$
 \hookrightarrow if constant, get Frank's theory]

Spont. stretch $\alpha non + \frac{1}{\sqrt{\alpha}} (I - non)$
 $\alpha = Q^{1/3} > 1, \frac{1}{\sqrt{\alpha}} = Q^{-1/6} < 1$

Incompressible $\det B = 1$

Energy minimized if $B = FF^T = \alpha^2 N + \frac{1}{\alpha} (I - N) =: L(n)$

Possible expression $\bar{W}(F, n) = \frac{1}{2} \mu [\text{tr}(BL^{-1}(n)) - 3]$

$\left[\begin{aligned} \det(BL^{-1}) &= 1 \\ \text{tr}(BL^{-1}) &\text{ minimized at value 3 by} \\ BL^{-1} &= I \\ \Rightarrow B &= L(n) \end{aligned} \right.$

Remarks

- Ref. config. ($F=I$) is the one the system would have if heated to isotropic case
- Spontaneous stretch in $F = L^{1/2}(n)$
- All this is really due to Warner-Terentjev (with PD's)

def $\int_{\Omega} \bar{W}(\nabla y, n) - \dots$ + BC of dirf & traction (not involving n)

inf $\int_{\Omega} \underbrace{\text{min}_{|n|=1} \bar{W}(\nabla y, n)}_{=: W(\nabla y)} - \dots$ + BC's ~~not involving~~

will mostly use this in the sequel

Some explicit formulas

$$L(u) = e^{2/3} N + e^{-1/3} (J - N)$$

$$\Rightarrow L^{-1}(u) = a^{-2/3} N + a^{1/3} (J - N) = a^{1/3} \left(J - \underbrace{\left(1 - \frac{1}{a}\right) N}_{> 0} \right)$$

$$BL^{-1}I = B \cdot L^{-1}$$

$$\bar{W}(F, u) = \frac{1}{2} \mu \left[B \cdot L^{-1}(u) - 3 \right] = \frac{1}{2} \mu a^{1/3} \left[\text{tr} B - \underbrace{\left(1 - \frac{1}{a}\right) \frac{B \cdot n \cdot n}{|n|^2}}_{> 0} - 3a^{-1/3} \right] \geq 0, = 0 \text{ for } B=L(u)$$

$$W(F) = \min_{|n|=1} \bar{W}(F, u) = \frac{1}{2} \mu a^{1/3} \left[\text{tr} B - \underbrace{\left(1 - \frac{1}{a}\right) \max_{|n|=1} \frac{B \cdot n \cdot n}{|n|^2}}_{= \lambda^2_{\max}(B)} - 3a^{-1/3} \right]$$

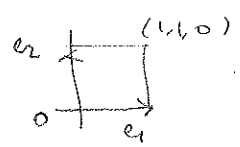
$n^* = \text{eig}_{\max}(B)$, max value of $B = FF^T$ achieved by

$$= \frac{1}{2} \mu e^{1/3} \left[\lambda^2_{\min}(F) + \lambda^2_{\text{mid}}(F) + \frac{1}{a} \lambda^2_{\max}(F) - 3a^{-1/3} \right]$$

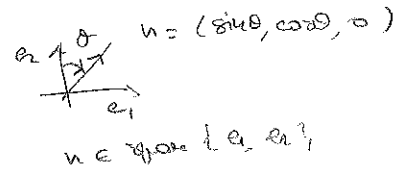
- J's are ISO and FI expressions
- Recover Neeth. for $a=1$, but have changed lower $|F|^2$ into nonconvex expression.

Energy landscape.

2d (plane - shear) perturbations of square. Shear associated with $n = e_2$



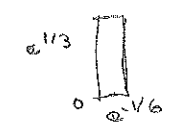
$$y(\theta) = 0 + Fx, \quad F = \begin{bmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$$



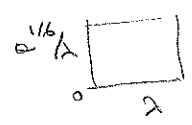
$\Omega = \text{unit sq. cube}$

Consider $\lambda \in [e^{-1/6}, e^{1/3}]$

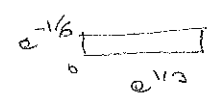
$$F(\lambda, 0) = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & a^{1/6}/\lambda & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$$



$$F(a^{-1/6}, 0) = L^{1/2}(e_2)$$

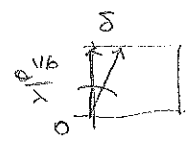


$$F(\lambda, 0)$$



$$F(a^{1/3}, 0) = L^{1/2}(e_1)$$

$$F(\lambda, \delta) = \begin{bmatrix} \lambda & \delta & 0 \\ 0 & a^{1/6}/\lambda & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$$



$$F(\lambda, \delta) e_2 = \begin{bmatrix} \delta \\ a^{1/6}/\lambda \\ 0 \end{bmatrix}$$

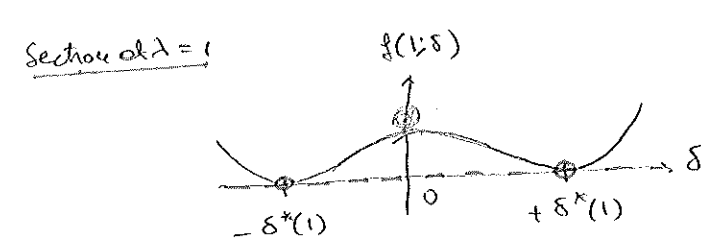
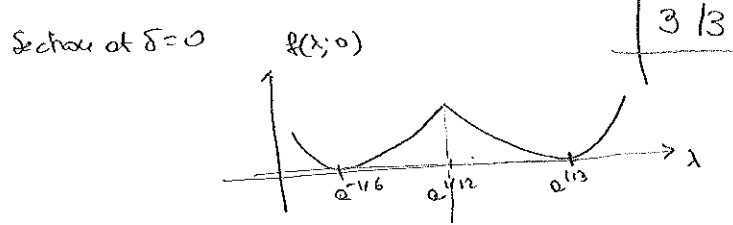
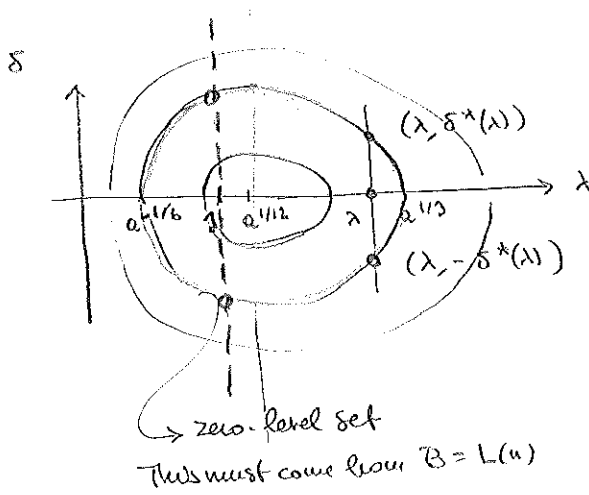
$$\text{shear} = \frac{\lambda}{a^{1/6}} \delta \quad (\text{shear amplitude})$$

$$B = FF^T = \begin{bmatrix} \lambda^2 + \delta^2 & \delta a^{1/6}/\lambda & 0 \\ \cdot & a^{1/3}/\lambda^2 & 0 \\ \cdot & \cdot & a^{-1/3} \end{bmatrix}$$

$$\bar{W}(F(\lambda, \delta), u(\theta)) = \bar{f}(\lambda, \delta, \theta) = \dots$$

$$\min_{\theta} \bar{W}(F(\lambda, \delta), u(\theta)) = W(F(\lambda, \delta)) = f(\lambda, \delta) = \dots$$

← Plot.



$$\text{tr } B(\lambda, \delta) = \lambda^2 + \delta^2 + \frac{a^{1/3}}{\lambda^2} + a^{-1/3}$$

$$\text{tr } L(n) = e^{2/3} + e^{-1/3} + e^{-1/3}$$

imposing equality, we obtain

$$\lambda^2 + \delta^2 + \frac{a^{1/3}}{\lambda^2} = e^{2/3} + e^{-1/3} \Rightarrow \delta^2 = \dots = \left(e^{2/3} - \lambda^2 \right) \left(1 - \frac{a^{-1/3}}{\lambda^2} \right)$$

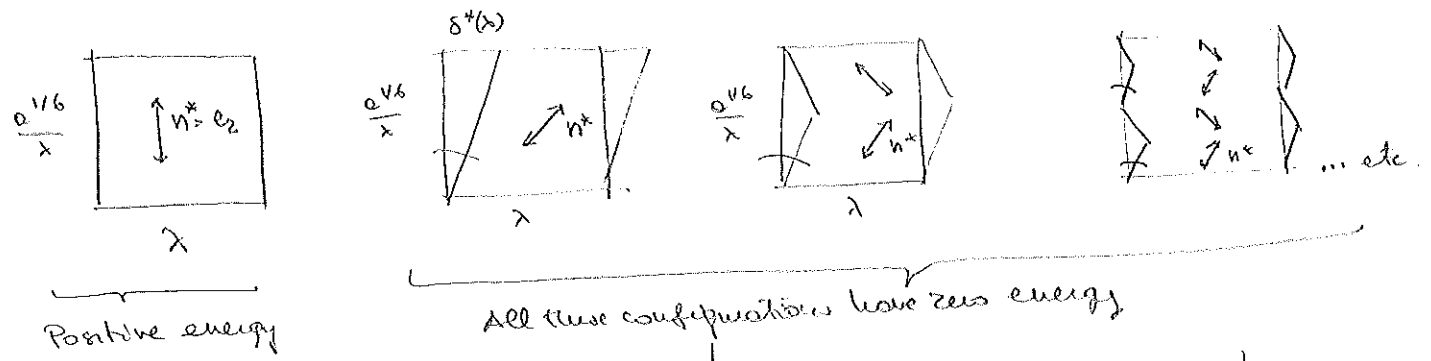
$$\delta^*(\lambda) = \left(1 - \frac{a^{-1/3}}{\lambda^2} \right)^{1/2} \left(e^{2/3} - \lambda^2 \right)^{1/2}$$

[this gives energy minima of horizontal lambda. will do this next time again in the future]

Use of the plot

Fix $\lambda \in [a^{-1/6}, a^{1/2}]$ and verify that, in this range $e_{\max}(B(\lambda, 0)) = n^* = e_2$ (EX)

The energy $\delta \mapsto f(\lambda; \delta)$ is even, hence stationary at $\delta=0$. This means that, at fixed λ , the state $\delta=0, \theta=0$ is an equilibrium. But $\frac{\partial^2}{\partial \delta^2} f(\lambda; \delta) \Big|_{\delta=0} < 0$ shows that this uniaxial state is unstable towards shears and shear banding.



[Idea: compress \square inside a box \square \approx accordion/compression pattern]

This explains the "stripe domain" instability observed in experiments. (optical contrast with transparent/opaque horizontal bands due to spatial oscillations of the nematic director).

A calculation in the same spirit by de Gennes (mid 80's) gave the impetus to experimental NEs (early 90's).

P.G. de Gennes' version: expand around $\delta = \theta = 0$, an equilibrium state w/ λ fixed.

[SKIP?]

$$\bar{f}(\lambda; \delta, \theta) = \bar{f}(\lambda; 0, 0) + \underbrace{\frac{\partial \bar{f}}{\partial \delta}}_{=0}(\lambda; 0, 0) \delta + \underbrace{\frac{\partial \bar{f}}{\partial \theta}}_{=0}(\lambda; 0, 0) \theta + \frac{1}{2} \left\{ \underbrace{\frac{\partial^2 \bar{f}}{\partial \delta^2}}_{G_{\delta\delta}}(\lambda; 0, 0) \delta^2 + 2 \underbrace{\frac{\partial^2 \bar{f}}{\partial \delta \partial \theta}}_{G_{\delta\theta}}(\lambda; 0, 0) \delta \theta + \underbrace{\frac{\partial^2 \bar{f}}{\partial \theta^2}}_{G_{\theta\theta}}(\lambda; 0, 0) \theta^2 \right\} + h.o.t.$$

$$G_{\theta\theta} = \mu a^{1/3} \left(\frac{a-1}{a} \right) \left(\frac{a^{1/3}}{\lambda^2} - \lambda^2 \right) > 0 \text{ if } \lambda < a^{1/6}$$

fixed stretching parameter

Find $\theta^*(\delta)$

(equil. value of θ , as a function of δ, λ . It depends on λ as well, but omit from notation.)

$$\frac{\partial}{\partial \theta} \frac{1}{2} \left\{ G_{\delta\delta} \delta^2 + 2 G_{\delta\theta} \delta \theta + G_{\theta\theta} \theta^2 \right\} = G_{\delta\theta} \delta + G_{\theta\theta} \theta = 0 \Rightarrow \theta^* = - \frac{G_{\delta\theta}}{G_{\theta\theta}} \delta$$

Plug back into \bar{f}

$$\bar{f}(\lambda; \delta, \theta^*(\delta)) = \frac{1}{2} \left\{ G_{\delta\delta} \delta^2 - 2 \frac{G_{\delta\theta}^2}{G_{\theta\theta}} \delta^2 + G_{\theta\theta} \frac{G_{\delta\theta}^2}{G_{\theta\theta}^2} \delta^2 \right\} + h.o.t.$$

$$\approx \frac{1}{2} \left\{ G_{\delta\delta} - \frac{G_{\delta\theta}^2}{G_{\theta\theta}} \right\} \delta^2$$

G_{eff}

$$G_{eff} = \mu a^{1/3} (1 - g(\lambda)) < 0 \text{ for } \lambda > a^{-1/6}$$

a strictly increasing function starting from $g(\lambda)|_{\lambda=0} = 1$

Compare with

$$\bar{f}(\lambda, \delta, \theta=0) \approx \frac{1}{2} G_{\delta\delta} \delta^2$$

$\mu a^{1/3} > 0$

$G_{eff} < G_{\delta\delta}$ always, because of elasto-neumatic coupling.

Conclude:

- Director mobility always decreases shear modulus: $G_{eff} < G_{\delta\delta}$
- On this basis, de Gennes proposed the need for θ 's (let's first speculated in early 90s) that a rubbery solid with embedded nematic mesogens could have interesting mech. properties because of soft modes arising from elasto-nematic coupling
- The cause for the instability $G_{eff} < 0$ is the mobility of the director, which reduces the effective shear modulus to zero or to negative values, as soon as λ enters the range $(a^{-1/6}, a^{1/6})$

In reality, one sees instabilities and vanishing of shear moduli only past a stretch threshold $\lambda_c > a^{-1/6}$.

Not surprising. There exist a preferred direction $n_0 = e_2$, the director substructure at crosslinking.

$$\bar{W}_\beta(F, n) = \frac{1}{2} \mu \left\{ (\text{tr } B L^{-1}(n) - 3) + \beta (\text{tr } C L^{-1}(n_0) - 3) \right\}, \quad \det B = \det C = 1$$

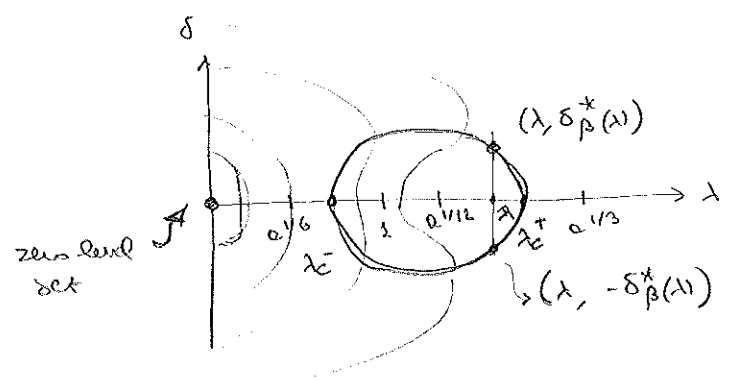
$\bar{W}_\beta \geq 0$, = 0 only if both $B = L(n)$ and $C = L(n_0)$

$B = L(n) \Rightarrow F = VR = L^{1/2}(n)R = \left[\alpha n \otimes n + \frac{1}{\sqrt{\alpha}} (I - n \otimes n) \right] R$ (EX)

$C = L(n_0) \Rightarrow F = QU = Q L^{1/2}(n_0) = Q \left[\alpha n_0 \otimes n_0 + \frac{1}{\sqrt{\alpha}} (I - n_0 \otimes n_0) \right]$

equality of RHSs $\Rightarrow Q = R$ and $n = \pm R n_0, F = R L^{1/2}(n_0)$

Energy landscape in (λ, δ) plane similar as before, except that region of nonconvexity and instabilities are shifted past λ_c .



$$\lambda_c = \lambda_c^- = \left(\frac{1+\beta}{\alpha+\beta} \right)^{1/2} a^{1/6}$$

$$\delta_\beta^*(\lambda) = \frac{1}{\lambda} \left(\frac{a^{1/3}}{\lambda_c^2} - \lambda^2 \right) (\lambda^2 - \lambda_c^2)^{1/2} \quad (\text{SKIP})$$

$$\lambda_c^+ = \frac{a^{1/6}}{\lambda_c}$$

Small strain theory

Assume that spontaneous distortions and Cauchy-Green strains are small perturbations of I

$$a^{1/3} = 1 + \gamma, \quad \gamma \ll 1$$

$$C = B = I + 2E, \quad |E| = \gamma \ll 1$$

Taylor expand upto γ^2 :

$$\frac{1}{2} \mu \left[(\det B)^{-1/3} B \cdot L^{-1}(n) - 3 \right] + \frac{1}{2} \mu \beta \left[(\det C)^{-1/3} C \cdot L^{-1}(n_0) - 3 \right] + \frac{\mu}{2} (\det(B^{1/2}) - 1)^2$$

$$\bar{\varphi}_\beta(E, n) = \mu |E_d - E_0(n)|^2 + \mu \beta |E_d - E_0(n_0)|^2 + \frac{\mu}{2} (\text{tr } E)^2$$

(unconstrained version)

$$\bar{\varphi}(E, n) = \mu |E - E_0(n)|^2 \quad \text{tr } E = 0$$

$$\bar{\varphi}_\beta(E, n) = \bar{\varphi}(E, n) + \mu \beta |E - E_0(n_0)|^2$$

where $E_0(n) = \frac{3}{2} \gamma (n \otimes n - \frac{1}{3} I)$

$$= \frac{3}{2} \frac{\delta}{a} s(n \otimes n - \frac{1}{3} I) = \gamma^2 Q$$

$$= (n \otimes n - \frac{\delta}{2} (I - n \otimes n))$$

$$|E_0(n)| = (\gamma^2 + 2 \frac{\delta^2}{a})^{1/2} = \sqrt{\frac{3}{2}} \delta$$

As n varies S^2 , $E_0(n)$ varies spherically, locally, uniaxial tensors of magnitude $\sqrt{\frac{3}{2}} \delta$

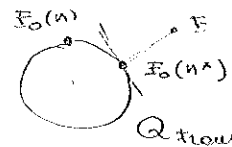
$\{ E \in M_{sym}^{3 \times 3}, \text{tr } E = 0, \text{ uniaxial, } |E| = \frac{\sqrt{3}}{2} \gamma \} =: \mathcal{Q} \text{ trace}$

Geometric structure of the energy landscape (case $\text{tr } E = 0$)

$$\bar{\varphi}(E, n) = \mu |E - E_0(n)|^2$$

$$\varphi(E) = \min_{|n|=1} \mu |E - E_0(n)|^2$$

$$= \mu \text{dist}^2(E, \mathcal{Q}_{\text{trunc}})$$



$\mathcal{Q}_{\text{trunc}} = \{ \text{eigen, traceless, unit-determinant tensor of magnitude } \sqrt{\frac{3}{2}} \}$

$\bar{\varphi}$ penalizes relative deformations $E^e = E - E_0(n)$

Looking back at nonlinear energy

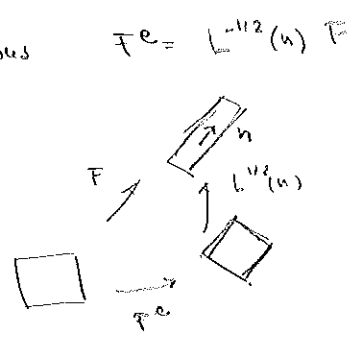
$$FF^T L^{-1}(n) \cdot I = L^{-1/2} F F^T L^{-1/2}(n) \cdot I$$

$$= \underbrace{(L^{-1/2} F)}_{F^e} \underbrace{(L^{-1/2} F)^T}_{F^{eT}} \cdot I = \text{tr}(F^e F^{eT})$$

(SUP)

Nonlinear energy penalizes "relative" deformations

$$\frac{1}{2} \mu [\text{tr}(F^e F^{eT}) - 3]$$



$$F = L^{1/2}(n) F^e$$

Many of the things we'll discover by analyzing the geometrically-linear theory have close analogs in the geometrically nonlinear theory.

Energy landscape in small strain theory

$n \in \text{span}\{e_1, e_2\}$

2d part of $\mathbb{E}_0(e_n)$: $\mathbb{E} = \mathbb{E}_0(e_n) + \begin{bmatrix} F & 0 \\ 0 & 0 \end{bmatrix}$

$\text{tr} \mathbb{E} = 0 \Rightarrow \text{tr} F = 0$

$$= \frac{3}{2} \gamma \begin{bmatrix} -1/3 & & \\ & 2/3 & \\ & & -1/3 \end{bmatrix} + \frac{3}{2} \gamma \begin{bmatrix} \epsilon & \delta & 0 \\ \delta & -\epsilon & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \frac{3}{2} \gamma \begin{bmatrix} \epsilon - 1/3 & \delta & 0 \\ \delta & 2/3 - \epsilon & 0 \\ 0 & 0 & -1/3 \end{bmatrix}$$

$\epsilon = 0, \delta = 0 \rightarrow \mathbb{E}_0(e_n)$
 $\epsilon = 1, \delta = 0 \rightarrow \mathbb{E}_0(e_1)$

$\bar{\varphi}(\epsilon, n) = \mu |\epsilon - \mathbb{E}_0(n)|^2$

$\bar{\varphi}_\beta(\epsilon, n) = \bar{\varphi}(\epsilon, n) + \mu \beta |\epsilon - \mathbb{E}_0(e_n)|^2$

$\varphi(\epsilon) = \min_{n=1} \mu |\epsilon - \mathbb{E}_0(n)|^2 = \mu \left[(\omega_{\max}(\epsilon) - \gamma)^2 + (\omega_{\min} + \gamma/2)^2 + (\omega_{\min} + \delta/2)^2 \right]$

2d version: $\mathbb{E} = \mathbb{E}_0(e_2) + \begin{bmatrix} F & 0 \\ 0 & 0 \end{bmatrix}$

$\bar{f}(F, n) = \mu |\mathbb{E}'_0(e_2) + F - \mathbb{E}'_0(n)|^2$

$f(F) = \min_{n=1} \bar{f}(F, n) = 2\mu \left[\omega_{\max}(\mathbb{E}'_0(e_2) + F) - \gamma \right]^2$

$f_\beta(F) = f(F) + \beta \mu |F|^2$

Define and plot

$\tilde{f}(\epsilon, \delta) = f(F(\epsilon, \delta)) = 2\mu (\omega_{\max} - \gamma)^2 = \dots \dots \text{plot} \dots$

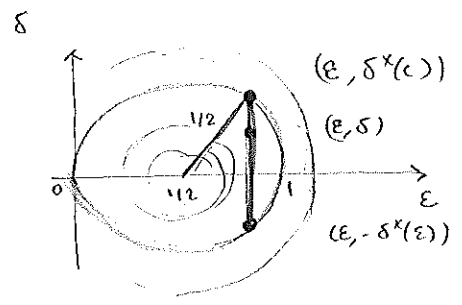
$\left[\begin{aligned} &= \frac{9}{2} \mu \gamma^2 \left(r(\epsilon, \delta) - \frac{1}{2} \right)^2 \\ &\quad \uparrow \\ &|(\epsilon, \delta) - (1/2, 0)| = \sqrt{(\epsilon - 1/2)^2 + \delta^2} \end{aligned} \right]$

$\tilde{f}_\beta(\epsilon, \delta) = f_\beta(F(\epsilon, \delta)) = \tilde{f}(\epsilon, \delta) + \beta \mu |F|^2$
 $\frac{9}{2} \gamma^2 (\epsilon^2 + \delta^2)$

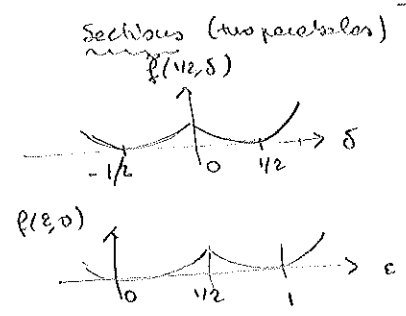
$= \dots \dots \text{plot} \dots$

$= \frac{9}{2} \mu \gamma^2 \left[(1+\beta) \left(r(\epsilon, \delta) - \frac{1}{2} \frac{1}{1+\beta} \right)^2 + \beta \left(\epsilon - \frac{1}{4} \frac{\beta}{1+\beta} \right) \right]$

isotropic case $f(\epsilon, \delta)$

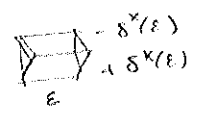


$$\delta^*(\epsilon) = \sqrt{\left(\frac{1}{2}\right)^2 - \left(\epsilon - \frac{1}{2}\right)^2}$$

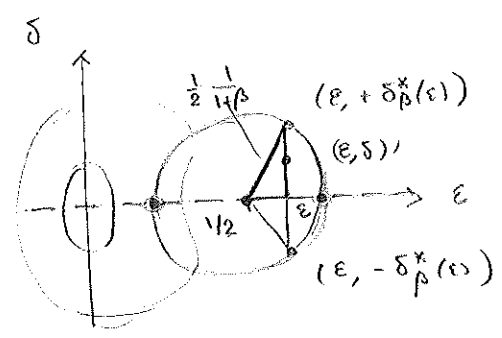


- level sets are circles because $w_{\text{non}}(\epsilon, \delta) = \text{const}$ over circles centered at $(1/2, 0)$
- zero level set is $w_{\text{non}} = r \Leftrightarrow r(\epsilon, \delta) = 1/2$

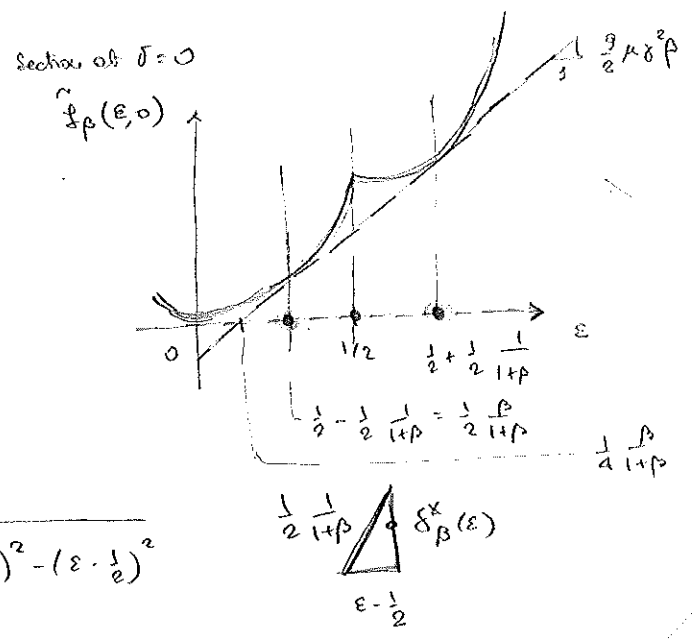
- the energy is proportional to the square of the distance from circle of radius $1/2$ centered at $(1/2, 0)$
- its convex envelope is obtained by replacing with distance from $\text{conv}(C)$
- can achieve it by "layering" $\pm \delta^*(\epsilon)$ at fixed ϵ



Anisotropic case $f_p(\epsilon, \delta)$



$$\delta^*_p(\epsilon) = \sqrt{\left(\frac{1}{2} \frac{1}{1+\beta}\right)^2 - \left(\epsilon - \frac{1}{2}\right)^2}$$



SUMMARY:

$$\tilde{f}_p^c(\epsilon, \delta) = \begin{cases} \tilde{f}_p(\epsilon, \delta) & \text{if } r \geq \frac{1}{2} \frac{1}{1+\beta} \\ \frac{1}{2} \mu \delta^2 & \text{else} \end{cases}$$

- this is a function proportional to distance from circle of radius $\frac{1}{2} \frac{1}{1+\beta}$ centered at $(1/2, 0)$
- + linear function
- Its convex envelope is obtained by replacing the first summand with distance from $\text{conv}(C_p)$.
- This can be achieved with $\tilde{f}_p^c(\epsilon, \delta) = \tilde{f}_p(\epsilon, \pm \delta^*_p(\epsilon))$

3. Relaxation results and quasiconvex envelopes

(4/1)

2d perturbations of state of spontaneous strain associated with $e_2 = n_0$.

Put directly []
in a convex
 $\tilde{f}_\beta^c(\epsilon, \delta) = \tilde{f}_\beta(\epsilon, \pm \delta^*)$

$$u(x) = \underbrace{u_1(x_1, x_2) e_1 + u_2(x_1, x_2) e_2}_{u'(x')} - \frac{\delta}{2} x_3 e_3$$

$$\nabla u = \left[\begin{array}{c|c} \nabla u' & 0 \\ \hline 0 & -\delta/2 \end{array} \right] = E_0(e_2) + \left[\begin{array}{c|c} \tau' & 0 \\ \hline 0 & 0 \end{array} \right]$$

$$E_0(e_2) = \frac{3}{2} \delta \begin{bmatrix} -1/3 & 0 & 0 \\ 0 & 2/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix}$$

$$\tau' = \nabla u' - E_0'(e_2) = \nabla' \left(u' - E_0'(e_2) x' \right) = \nabla' v'$$

(v' is the real unknown of the problem. Once we know v', we recover u' and hence u)

$$= \frac{1}{2} (\text{tr} F') \mathbb{1}' + (\text{sym} F')_d + \text{skew} F'$$

$$(\text{sym} F')_d = \frac{3}{2} \gamma \begin{bmatrix} \epsilon & \delta \\ \delta & -\epsilon \end{bmatrix} ; \quad \epsilon = \epsilon(F) = \frac{1}{\sqrt{2}} (F_{11} - F_{22}) \frac{\gamma'}{2\gamma}$$

$$\delta = \delta(F) = \frac{1}{\sqrt{2}} (F_{12} + F_{21}) \frac{\gamma'}{3\delta}$$

Drop primes from notation and work with 2x2 matrices.

$F \in M^{2 \times 2}$, arbitrary, define

$$\bar{h}_\beta(F, n) := \tilde{f}_\beta((\text{sym} F)_d, n) + \frac{k}{2} (\text{tr} F)^2$$

$$= \mu |E_0'(e_2) + (\text{sym} F)_d - E_0'(n)|^2 + \mu \beta |(\text{sym} F)_d|^2 + \frac{k}{2} (\text{tr} F)^2$$

$$h_\beta(F) = \min_{|n|=1} \bar{h}_\beta(F, n) = \tilde{f}_\beta((\text{sym} F)_d) + \frac{k}{2} (\text{tr} F)^2$$

Observe that, for $F \in \text{Sym}$, $\text{tr} F = 0$, we have $h_\beta(F) = \tilde{f}_\beta(F)$, so that h_β is an extension to non-symmetric, non-hessian matrices of our energy.

Since

$$k \nabla u = \underbrace{\text{tr} E_0'(e_2)}_{=0} + \text{tr} F = \text{div} v$$

the incompressible case " $k = +\infty$ " is obtained by enforcing constraint $\text{div} v = 0$. We'll worry about incompressibility after having dealt with compressible case.

$$\inf_{\substack{v \in H^1(\mathbb{R}^2; \mathbb{R}^2) \\ + \mathbb{R}^c}} H(v) := \int_{\mathbb{R}^2} h_\beta(\nabla v(x)) dx = \int_{\mathbb{R}^2} \tilde{f}_\beta((\text{sym} \nabla v)_d) + \frac{k}{2} (\text{div} v)^2$$

ill-posed problem because of non-convexity of \tilde{f}_β (min. sep. may develop increasingly fine periodic oscillations: stripe-domain instability).



\tilde{f}_β controlled by periodic bc tells how stripes are used below
 \Rightarrow classical relaxation thus apply.

$$\bar{H} = \sup \{ G : G \text{ is } H^1\text{-w.l.s.c.}, G \leq H \} \quad \text{relaxation of } H$$

$$\min_{v \in H^1} \bar{H}(v) = \inf_{v \in H^1} H(v)$$

minimizers of \bar{H} give inf of H , they represent w.l. limits of minimizing sequences of H

$$\bar{H}(v) = \inf_{k \rightarrow \infty} \left\{ \liminf_k H(v_k) : v_k \rightarrow v \text{ in } H^1(\Omega, \mathbb{R}^2) \right\}$$

$$H(v) = \int_{\Omega} h_p^{qc}(\nabla v(x)) dx$$

where

$$h_p^{qc}(T) = \inf_{w \in W_0^{1,p}} \left\{ \frac{1}{|w|} \int_w h_p(T + \nabla w(x)) dx \right\} \quad (\text{w arbitrary})$$

$$= \sup \{ g(T) : g \leq h_p, g \text{ quasiconvex} \}$$

Pb: what to do with this, given that there is no algorithmic characterization of quasiconvexity?

Some facts about convexity.

f quasiconvex at F if

$$f(F) \leq \frac{1}{|w|} \int_w f(F + \nabla w(x)) dx, \quad \forall w \in W_0^{1,\infty}(\Omega, \mathbb{R}^2) \quad (*)$$

Jensen's inequality for gradient perturbations of F with envelope F (so $\text{conv} \Rightarrow \text{qcconv}$)

• Analysis of material stability. Allude extension to w of F and ∂w gives energy minimum. If violated, f^{qc} gives the minimal energy the system can attain, compatibly with BC $y(x) = F_0$ on ∂w , by developing Lipschitz modulus μ in the interior of w .

f is rank-one convex if

$$f((1-\nu)\xi_1 + \nu\xi_2) \leq (1-\nu)f(\xi_1) + \nu f(\xi_2) \quad \forall \nu \in [0,1], \forall \xi_1, \xi_2 \in \mathbb{R}^{2 \times 2} \text{ with } \text{rank}(\xi_2 - \xi_1) \leq 1$$

rank-one convex hull of f

$$f^{rc}(\xi) = \sup \{ g(\xi) : g \leq f, g \text{ rc-convex} \}$$

$$f^c(\xi) = \sup \{ g(\xi) : g \leq f, g \text{ convex} \}$$

(so, weaker notion of convexity) out of qcconvexity. Use $w \equiv \xi_1 + \nu(\xi_2 - \xi_1)$ w.l. cut-off near ∂w . $\xi_2 = \xi_1 + a \otimes n, |H| \gg n$

Since $c \Rightarrow \text{qc} \Rightarrow \text{rc}$ (indirectly via rc , then qc , then c and

$$f^c \leq f^{qc} \leq f^{rc} \quad (**)$$

Contrary to f^{qc} , there are "algorithmic" characterizations for f^c and f^{rc} , so can at least bound f^{qc} . If the bounds match, we have f^{qc} .

$$f^c(\xi) = \inf \left\{ \sum_{i=1}^k \lambda_i f(\xi_i) : \sum \lambda_i \xi_i = \xi, \sum \lambda_i = 1, \lambda_i \in [0, 1] \right\}$$

where $k = N + 1$, if $\xi \in \mathbb{R}^N$

$$f^{*c}(\xi) = \inf_{k \geq 2} \left\{ \sum_{i=1}^k \lambda_i f(\xi_i) : \lambda_i, \xi_i \text{ define a laminate of "order } k \text{"} \right\}$$

def. by induction on k

$$\leq \inf \left\{ \dots \right\}$$

"condition H_k "
Do. analogue

$$= \inf \left\{ (1-\nu)f(\xi_1) + \nu f(\xi_2), (1-\nu)\xi_1 + \nu\xi_2 = \xi, \nu \in (0, 1), \text{conv}(\xi_2 - \xi_1) \leq 1 \right\}$$

"see 2"



Recall, for $F \in M^{2 \times 2}$

$$h_p(F) = f_p(\text{sym} F) + \frac{k}{2} (\text{tr} F)^2$$

$$\varepsilon = \frac{1}{2\delta} (F_{11} - F_{22})$$

$$\delta = \frac{1}{2\delta} (F_{12} + F_{21})$$

Define

$$\tilde{h}_p(\varepsilon, \delta, \text{tr} F) := \tilde{f}_p(\varepsilon, \delta) + \frac{k}{2} (\text{tr} F)^2$$

$$\tilde{j}_p(\varepsilon, \delta, \text{tr} F) := \tilde{f}_p^c(\varepsilon, \delta) + \frac{k}{2} (\text{tr} F)^2$$

$$j_p(F) := \tilde{j}_p(\varepsilon(F), \delta(F), \text{tr} F)$$

Theorem (Convex, DS) $h_p^{qc} = h_p^c = j_p$

Proof To show

$$(h_p)^{rc} \leq j_p \leq (h_p)^c \quad (*)$$

since by (**)

$$(h_p)^c \leq (h_p)^{qc} \leq (h_p)^{rc}$$

and then (*) would imply not all are =, and then it follows.

Second inequality easy, because

$$\tilde{j}_p \leq \tilde{h}_p \Big|_{\substack{\text{convex} \\ \text{}}} \Rightarrow j_p \leq (h_p)^c$$

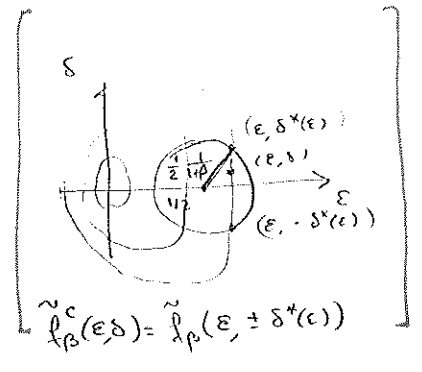
we are left to show that $(h_p)^{rc} \leq j_p$

Since $(h_p)^{rc} \leq h_p$, at all F where $h_p = j_p$ then it is nothing to prove

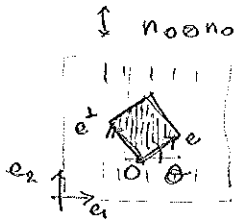
Conclude at $h_p \neq j_p$, i.e. where $\tilde{f}_p^c \neq \tilde{f}_p$, i.e. where

$$r(\varepsilon, \delta) < \frac{1}{2} \frac{1}{1+\beta}$$

where we use a laminate construction.

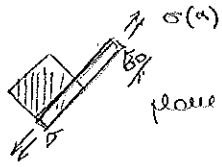


• stress-strain response in conditions of affine deformations.



$$e = (\cos\theta, \sin\theta)$$

$$e^+ = (-\sin\theta, \cos\theta)$$

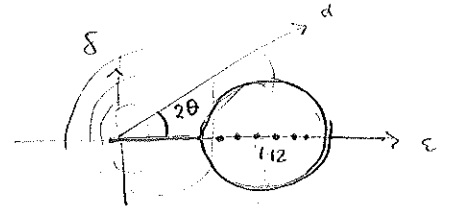


plane strain extension along e .

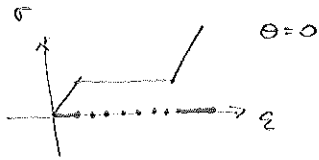
$$\frac{3}{2} \delta \alpha (e \otimes e - e^+ \otimes e^+) = \Delta E$$

$$e(\Delta E) = \alpha \cos 2\theta$$

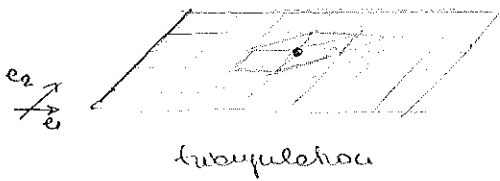
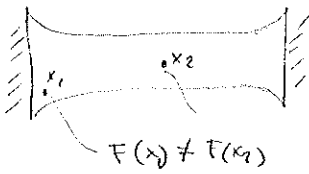
$$\delta(\Delta E) = \alpha \sin 2\theta$$



Use the of plane extended to obtain $\sigma(\alpha) = \frac{d}{d\alpha} \int_{\Omega} \rho^c(\epsilon(\alpha), \delta(\alpha))$



• stress-strain response in conditions of heterogeneous deformations, through "multiscale" finite elements



contact problem

piecewise linear basis functions.

If we use $W^{qc}(F)$ instead of $W(F)$, have accounted correctly for the asymptotics of energy minimizing rates, including microstructures, without having to resolve their kinematics explicitly.

Some of this features can be recovered from knowledge of the F_i 's set.

$$W^{qc}(\sum \lambda_i F_i) = \sum \lambda_i W(F_i)$$

• Other materials: coupling between elastic stretch and other tensor/vector variable: piezoelectrics, ferroelectrics, magnetic shape-memory,

Microstructures in nematic elastomers: modeling, analysis, and numerical simulation.

Antonio DeSimone

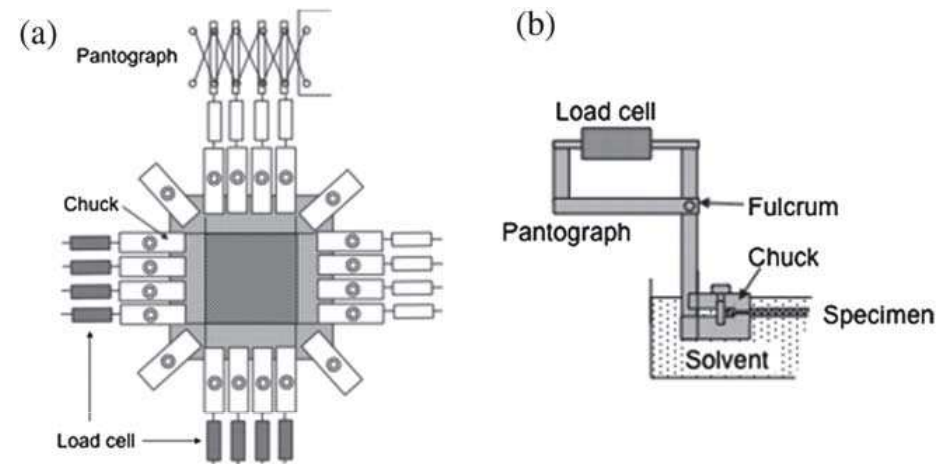
SISSA
International School for Advanced Studies
Trieste, Italy



<http://people.sissa.it/~desimone/>

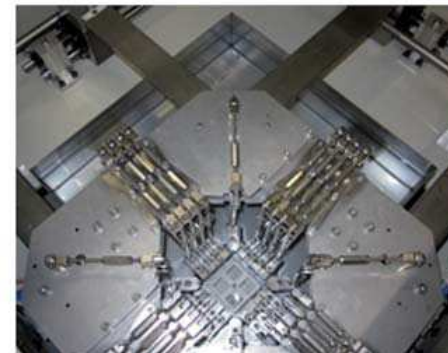
Sixth Summer School in Analysis and Applied Mathematics, Rome 20-24, 2011

Biaxial stretching experiments on soft sheets



Urayama_c0sm00955e.mov

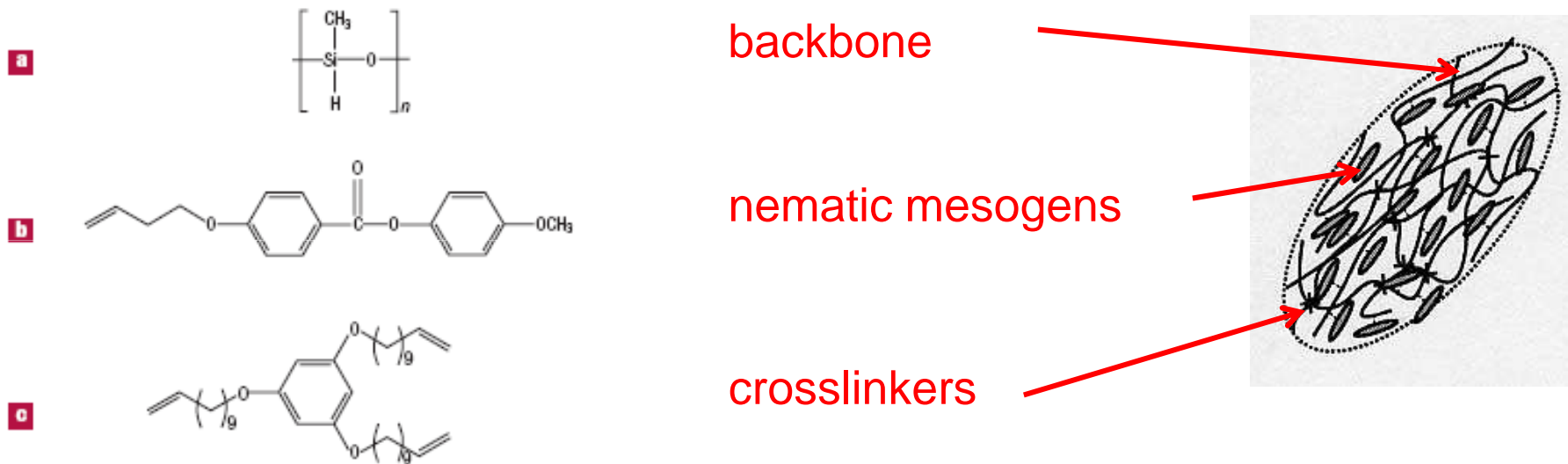
(c)



(K. Urayama)

What are Nematic Elastomers?

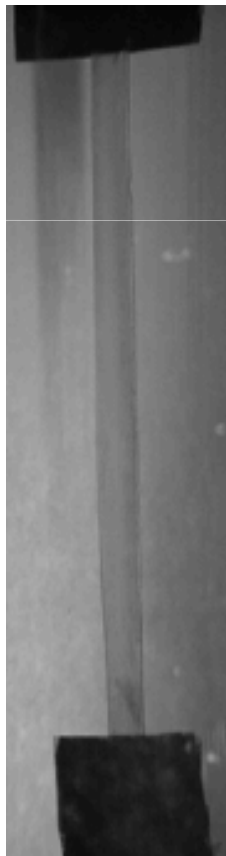
Cross-linked networks of polymeric chains containing nematic mesogens



They combine optical properties and orientational DOFs typical of nematic LCs
 (Frank curvature elasticity, dielectric anisotropy)
 with translational DOFs of an elastic solid
 (rubber elasticity)

Isotropic-to-Nematic Phase Transformation: spontaneous (Bain) strain

Cross-linked networks of polymeric chains containing nematic mesogens:
alignment of mesogens along average direction \mathbf{n}
induces spontaneous distortion of chains



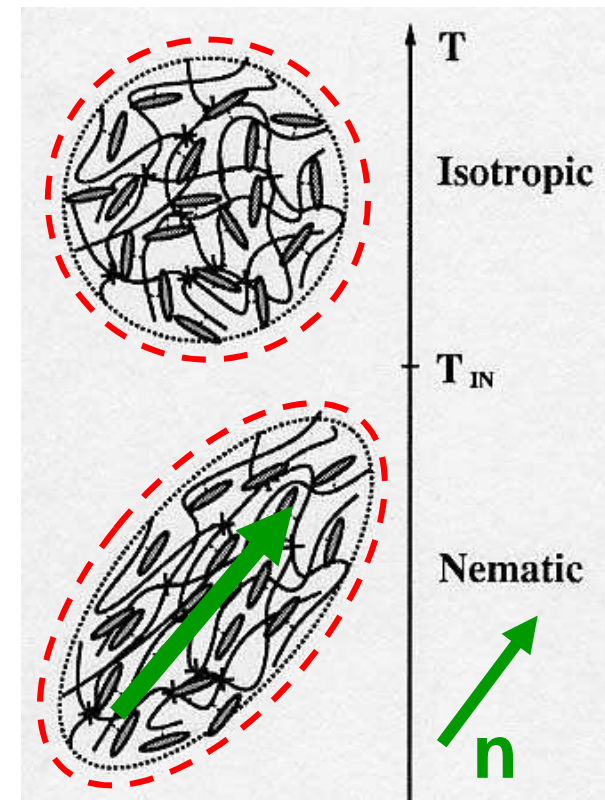
Spontaneous distortion :

$$F_n = a^{1/3} \mathbf{n} \otimes \mathbf{n} + a^{-1/6} (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$$

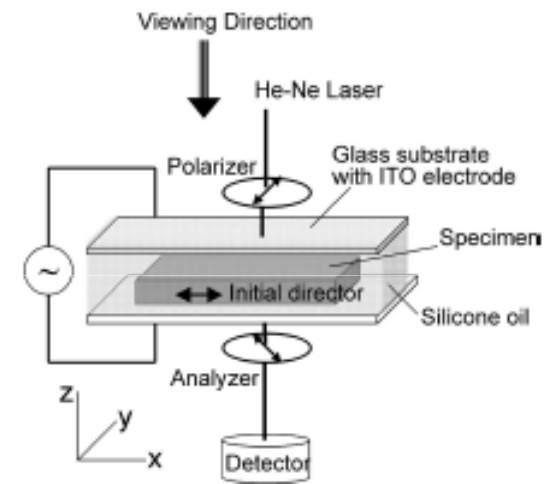
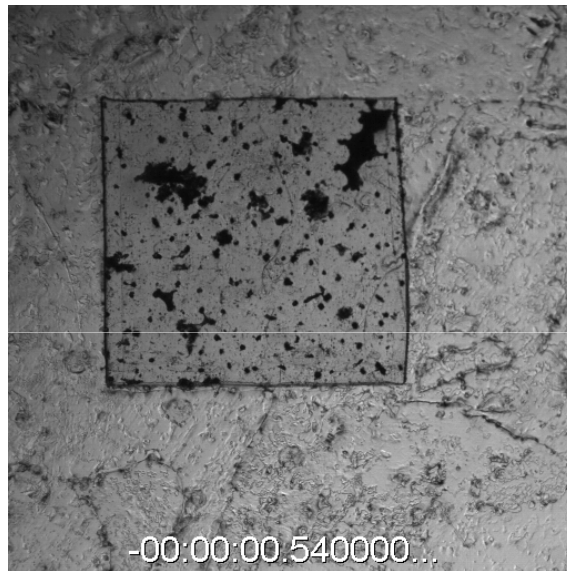
a volume preserving uniaxial extension
along \mathbf{n} of magnitude $a^{1/3} \geq 1$ ($a > 1$)

\mathbf{n} nematic director, $|\mathbf{n}|=1$

(H. Finkelmann)



Apply electric field to turn nematic director and spontaneous distortion

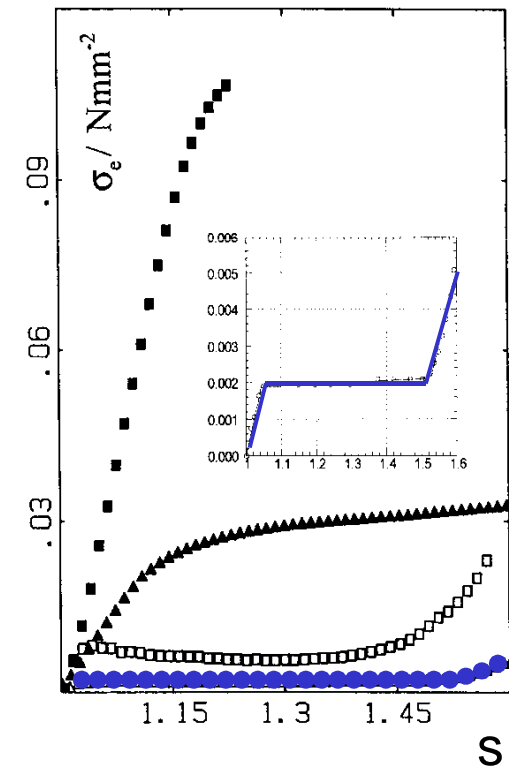
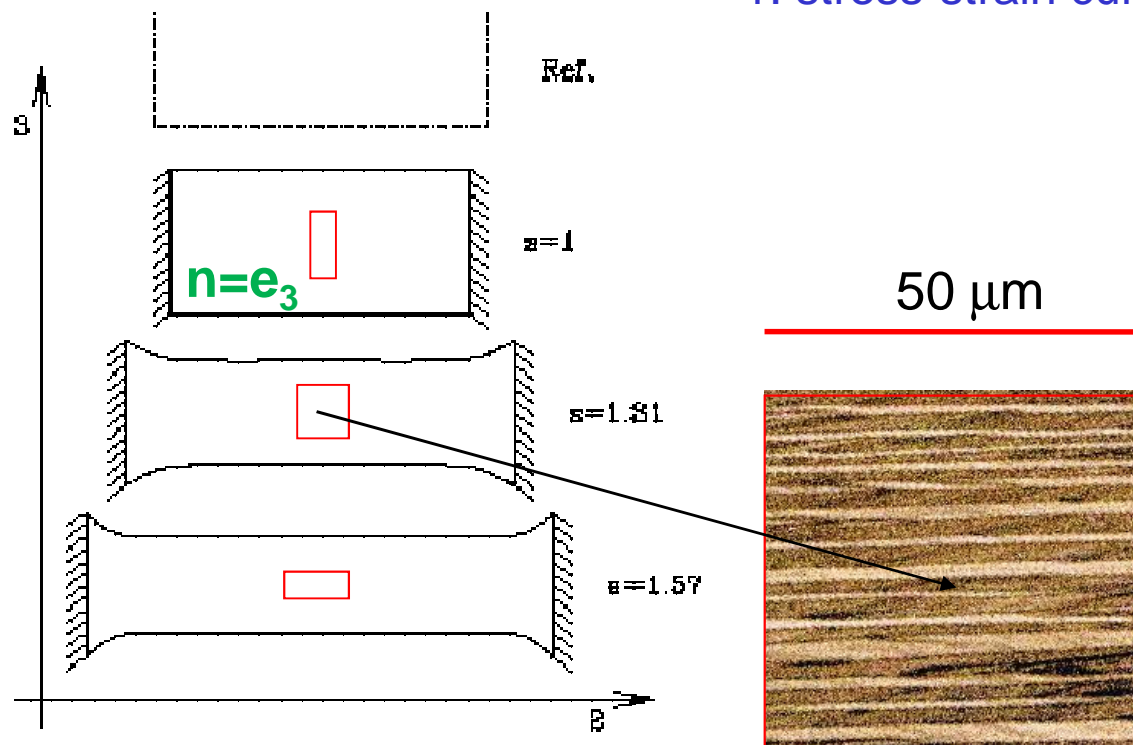


Purely mechanical stretching

Fixed temperature in the nematic phase.

Initial configuration: $s=1$, $n=e_3$. Stretch along e_2 with rigid clamps:

1: stress-strain curve has plateau (soft elasticity)

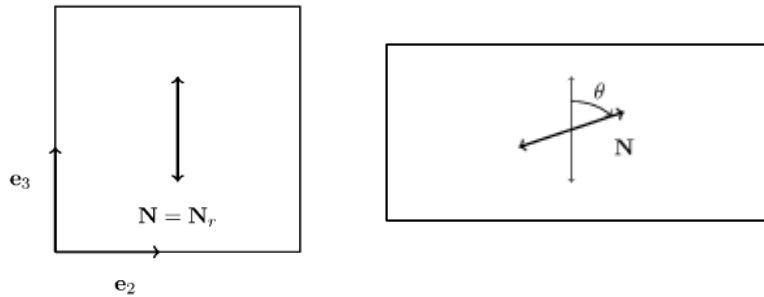


(H. Finkelmann, 95)

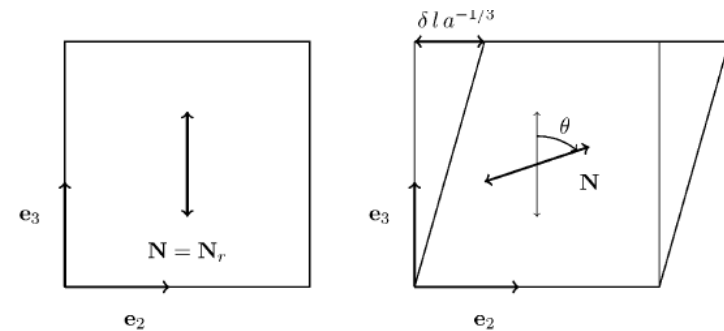
2: non-uniform director reorientation (stripe-domain instability)

Explore energy landscape through homogeneous stretch and shear: instabilities

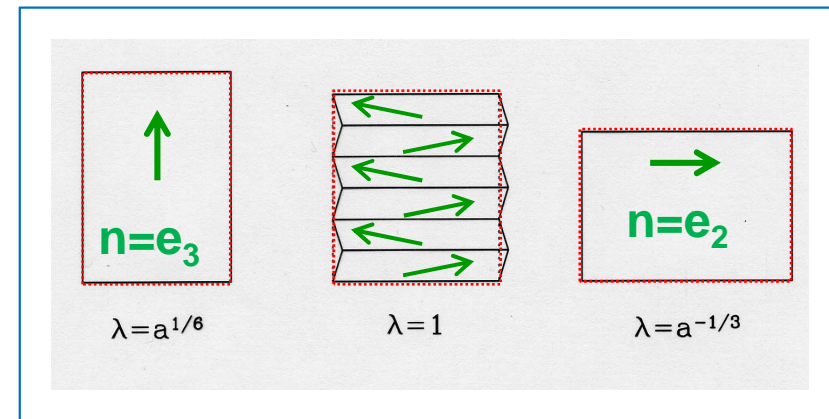
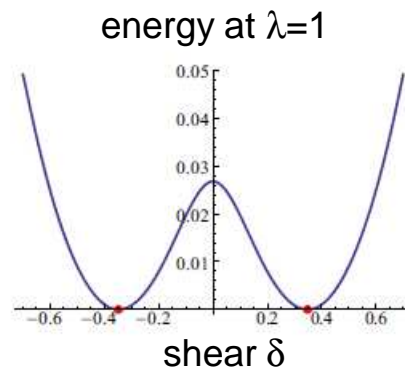
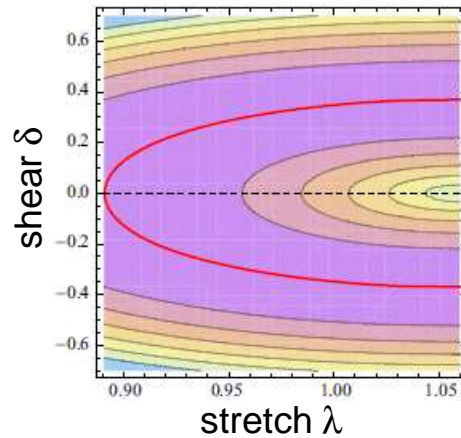
Stretch by λ



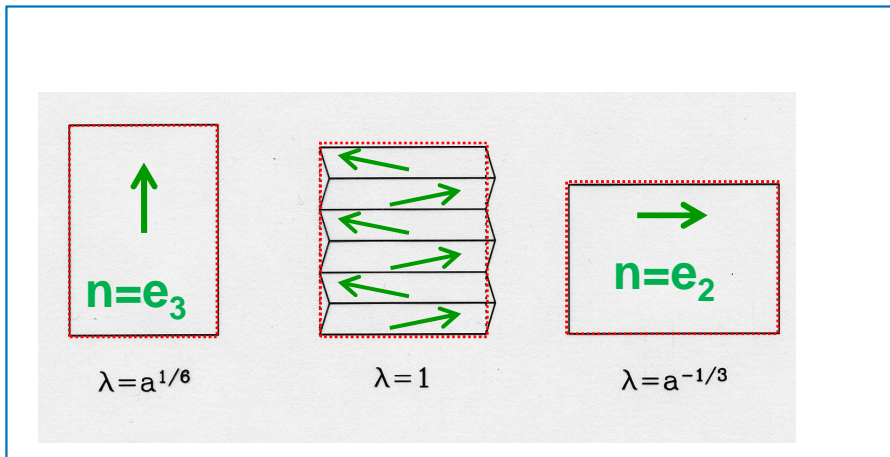
Shear by δ



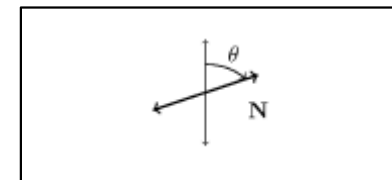
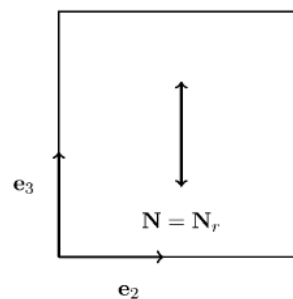
Min $W(F,n)$ (isotropic)
n



Similar instabilities for anisotropic energy

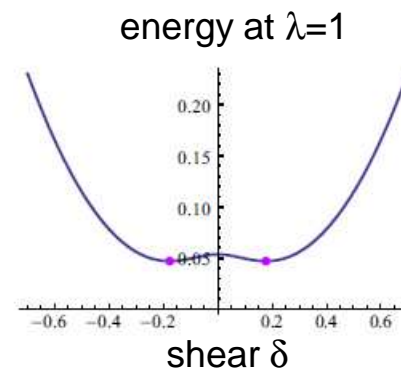
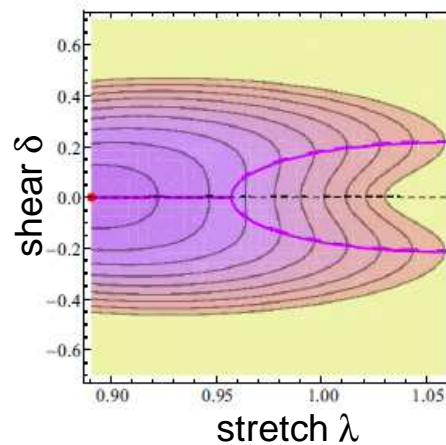
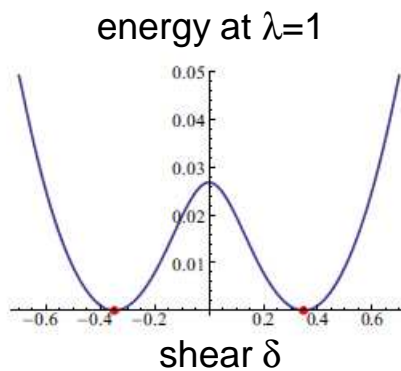
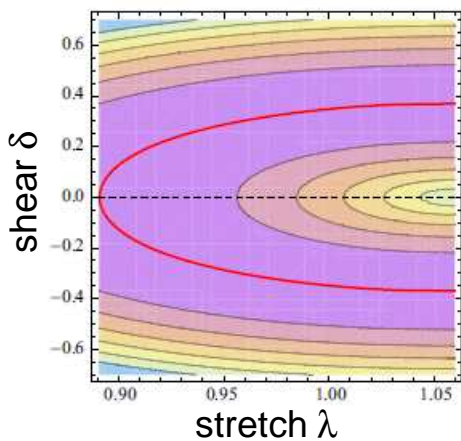


Stretch by λ



Min $W(F, n)$ (isotropic)
n

Min $W_\beta(F, n)$ (anisotropic)
n



Can use small strain theory as well

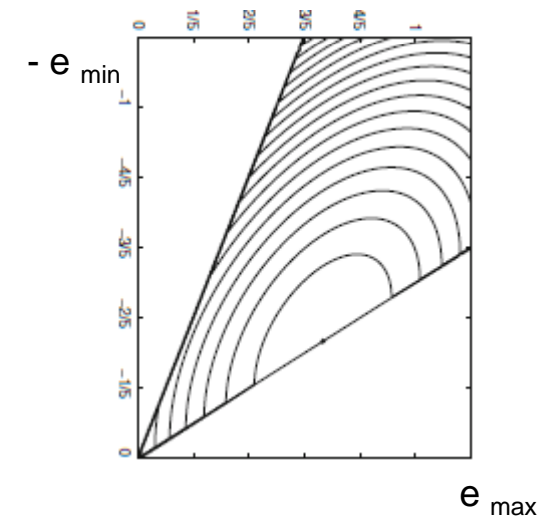
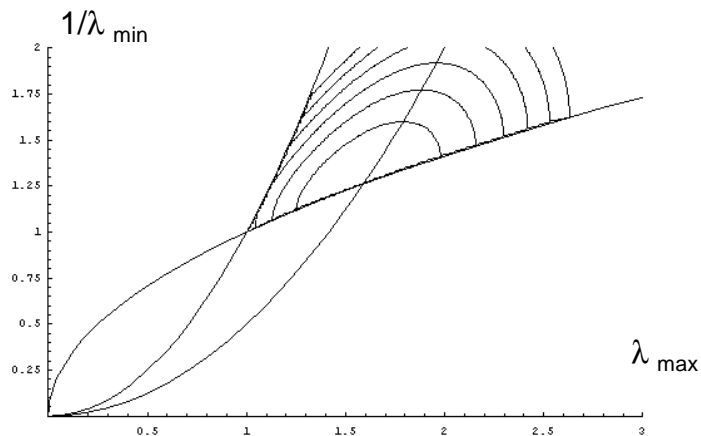
$$a^{1/3} = 1 + \gamma, \quad \gamma \ll 1$$

measures spontaneous stretch along n

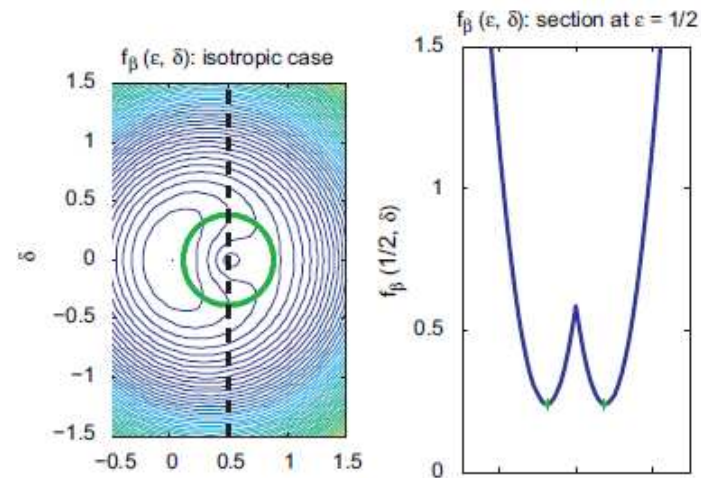
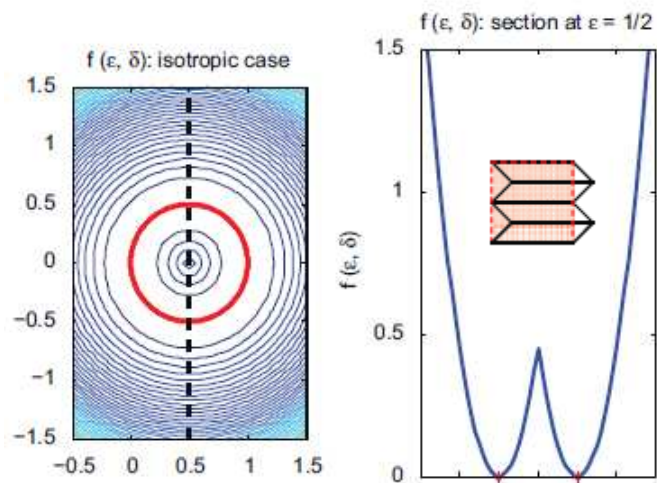
$$F_n = a^{1/3} n \otimes n + a^{-1/6} (I - n \otimes n) \quad \longrightarrow \quad I + E_0(n)$$

$$E_0(n) = \frac{3}{2} \gamma (n \otimes n - \frac{1}{3} I)$$

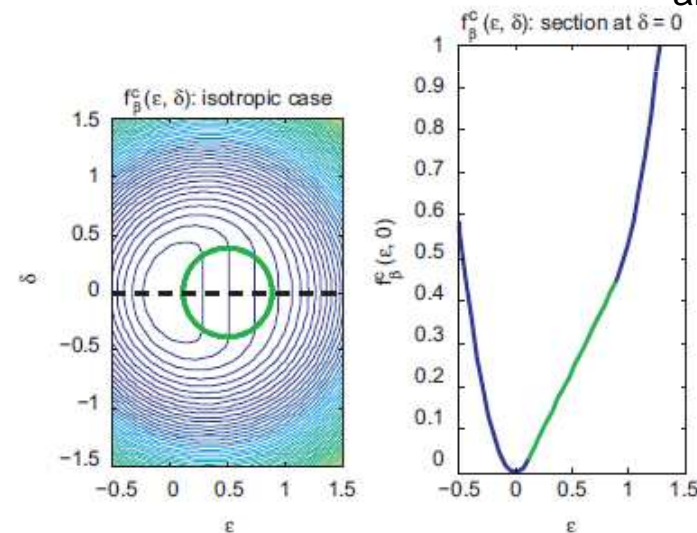
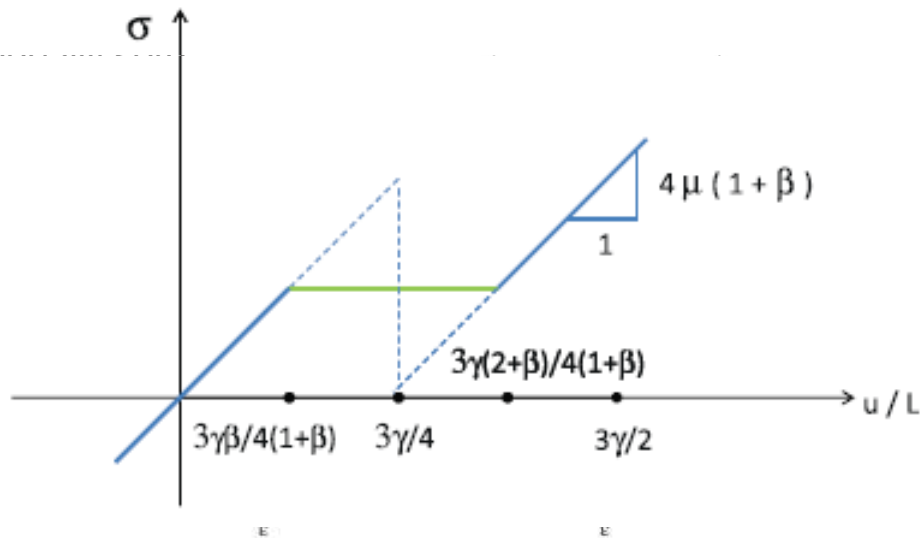
$$W(F, n) = \frac{1}{2} \mu (F F^T) \cdot (F_n F_n^T)^{-1} \quad \longrightarrow \quad \mu |E - E_0(n)|^2$$



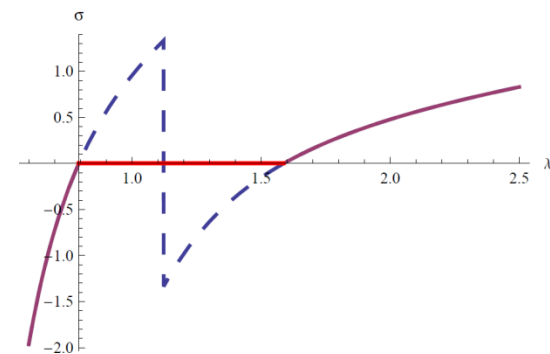
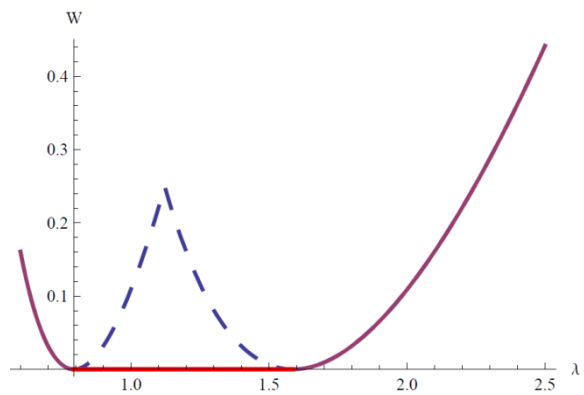
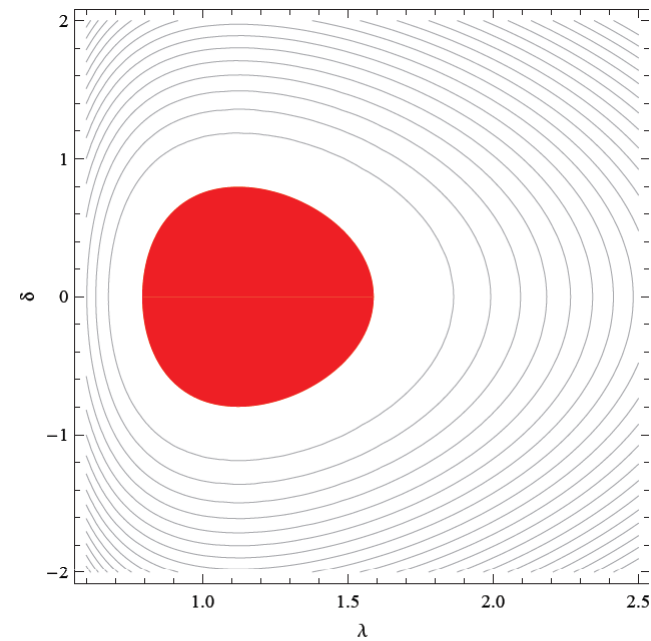
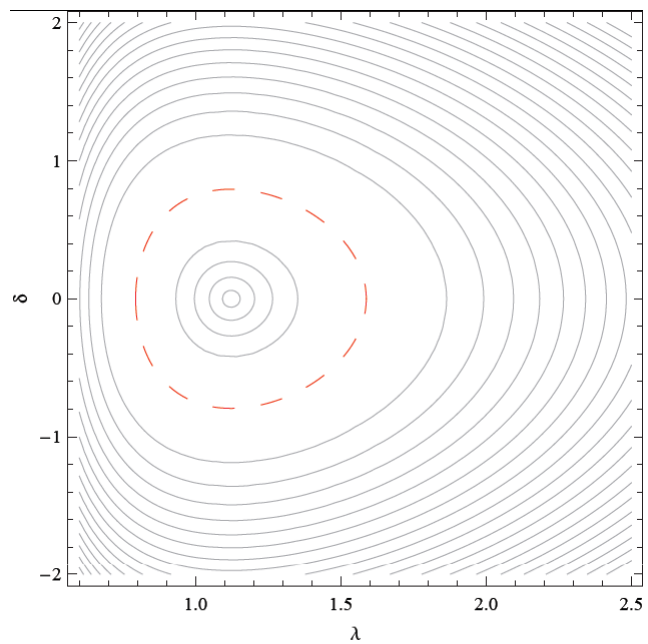
QC envelopes (plane strain, extension-shear)



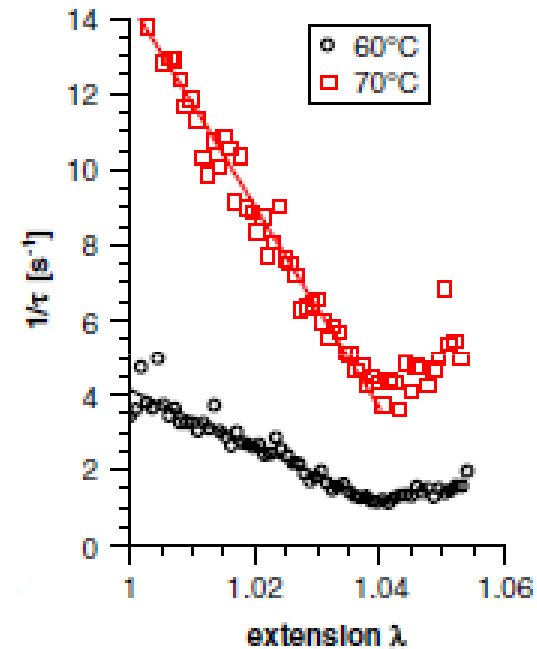
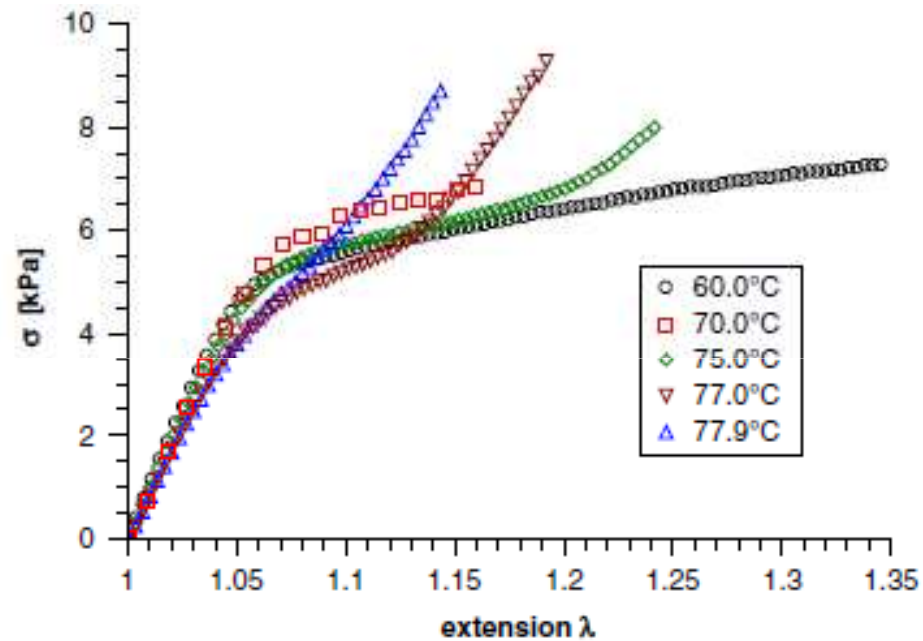
anisotropic



Finite elasticity (isotropic, plane strain)

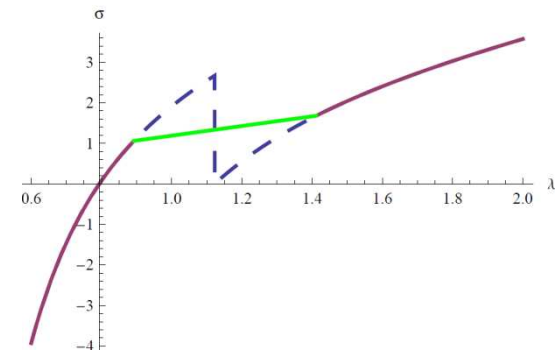
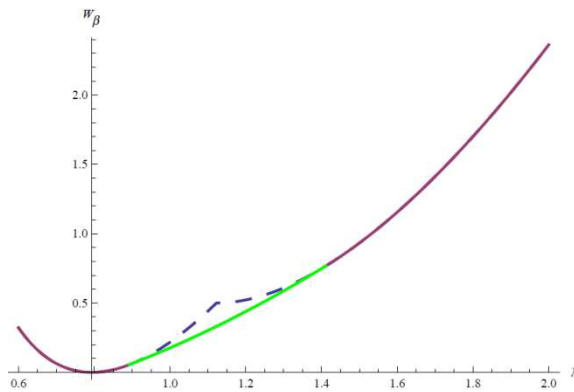
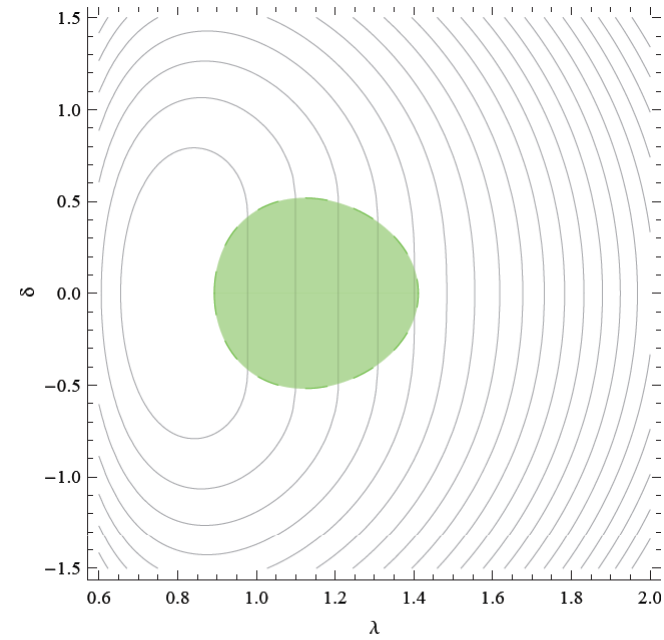
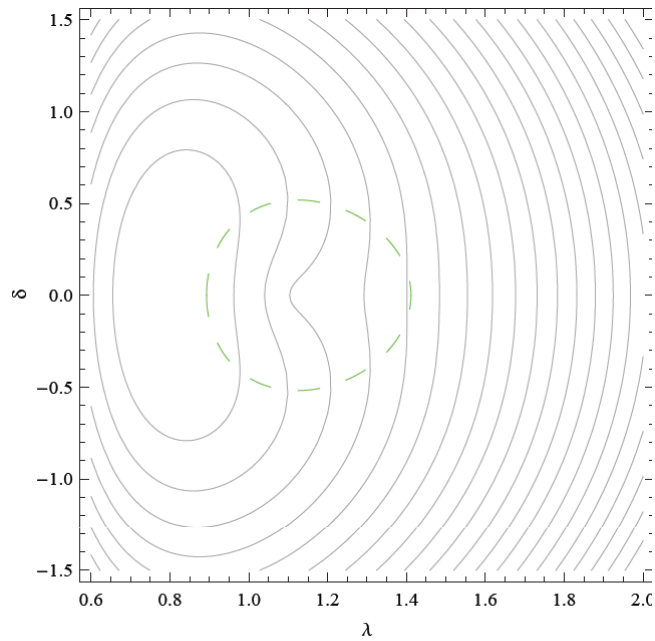


Soft response to stretch and vanishing of shear modulus after threshold stretch

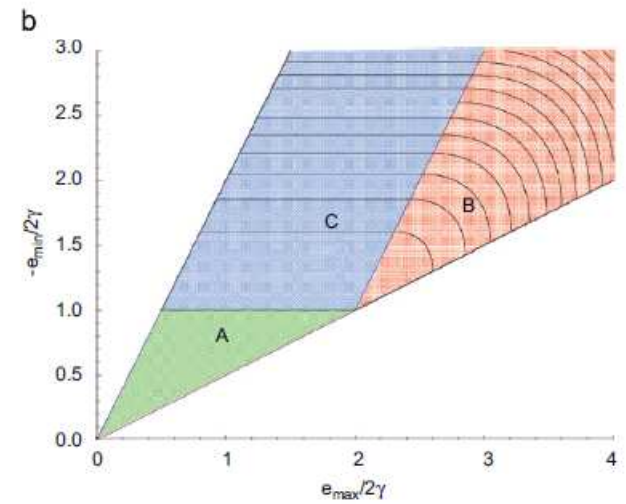
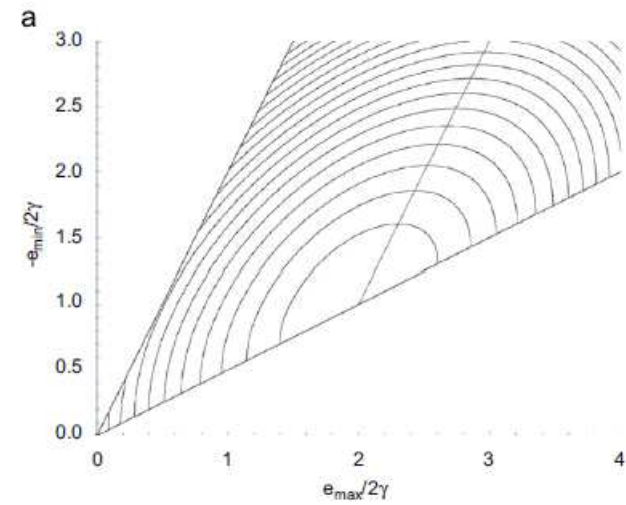
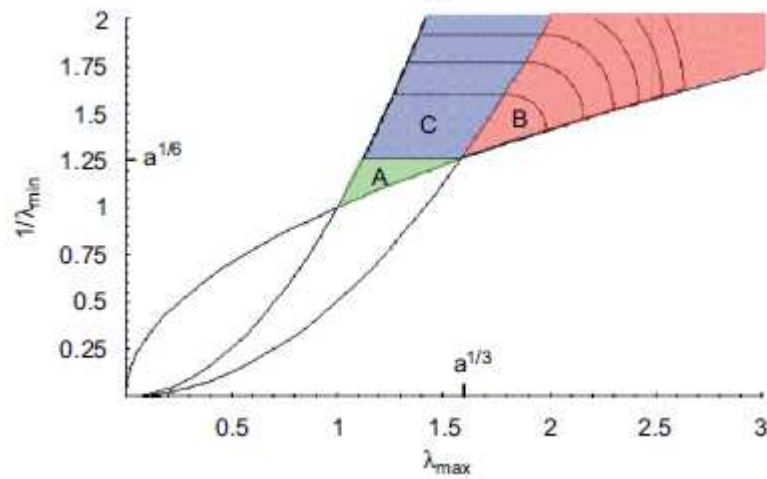
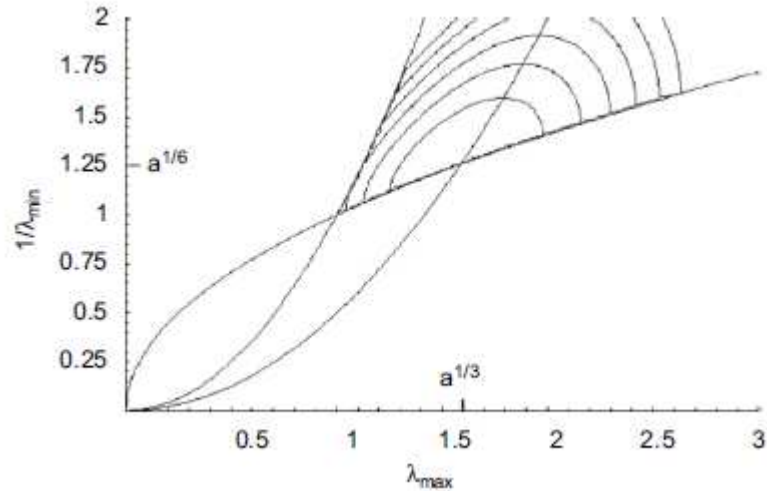


(M. Copic)

Finite elasticity (anisotropic, plane strain)



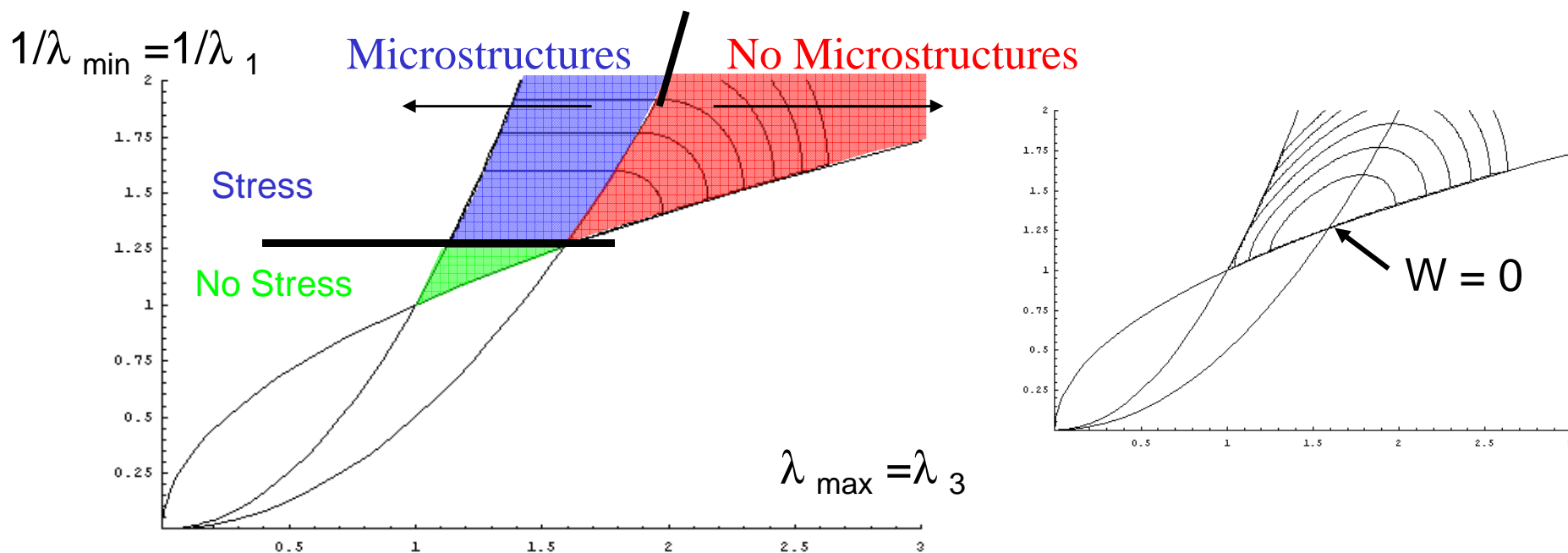
QC envelopes (3d, isotropic)



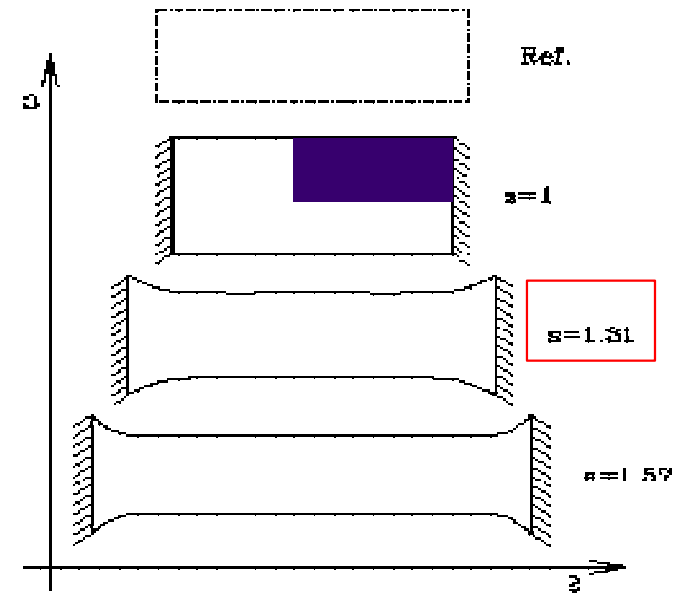
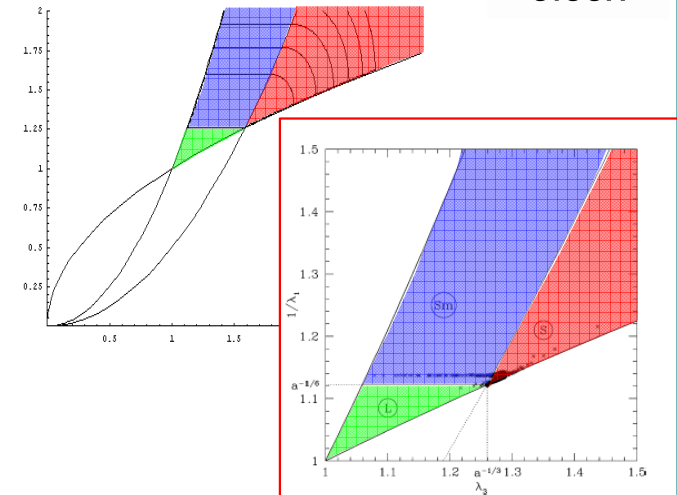
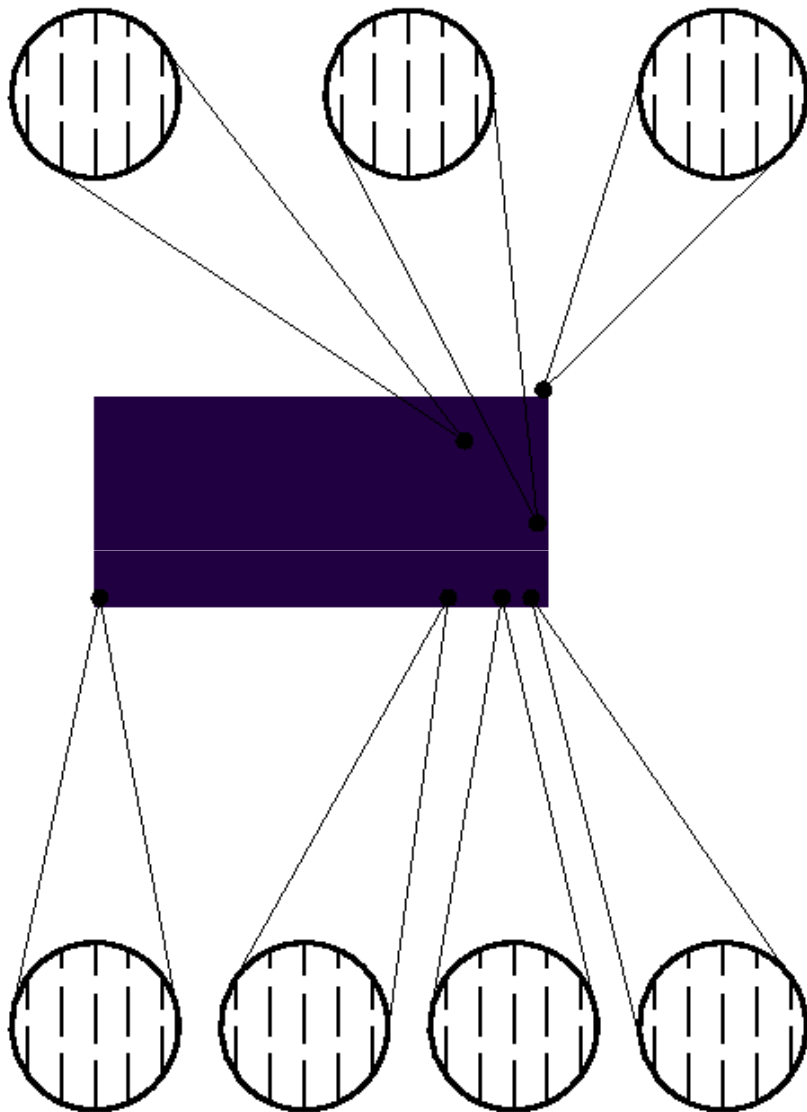
The quasi-convexified energy W^{qc}

$$W^{qc}(F) = \begin{cases} 0 & \text{(phase L) if } \lambda_1 \geq a^{1/6} \\ W(F) & \text{(phase S) if } a^{1/2} \lambda_3^2 \lambda_1 > 1 \\ \lambda_1^2 + 2a^{1/2} \lambda_1^{-1} - 3a^{1/3} & \text{(phase I or Sm) else} \end{cases}$$

if $\det F = 1$, $W^{qc}(F) = +\infty$ if $\det F \neq 1$.

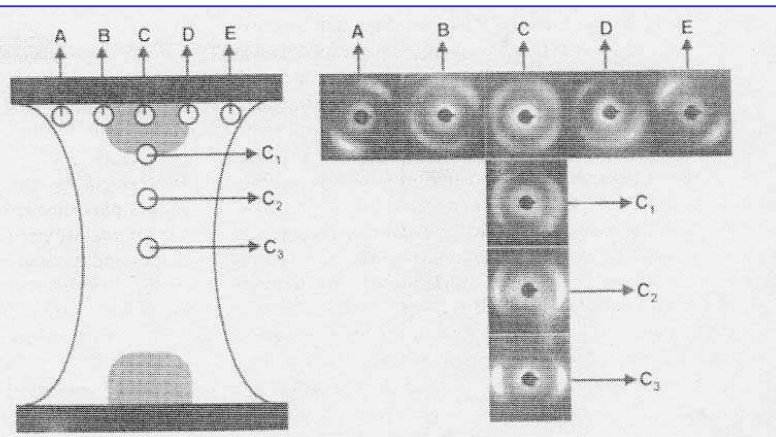
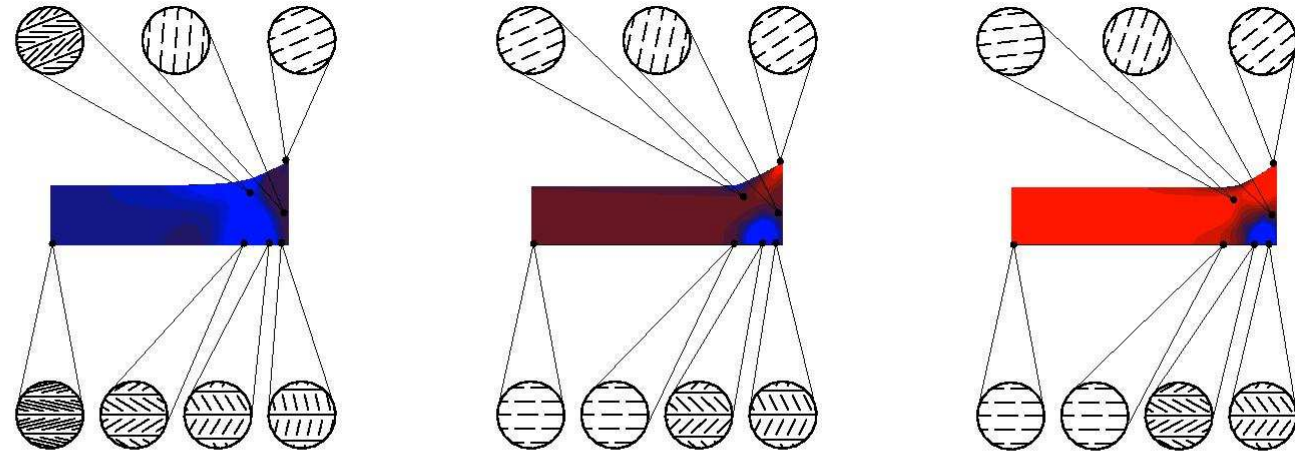


Use W^{qc} in numerical stretching experiment

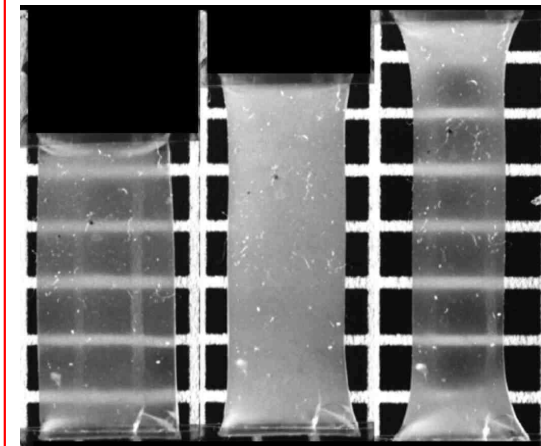


Theory vs. Experiment

Multiscale numerics

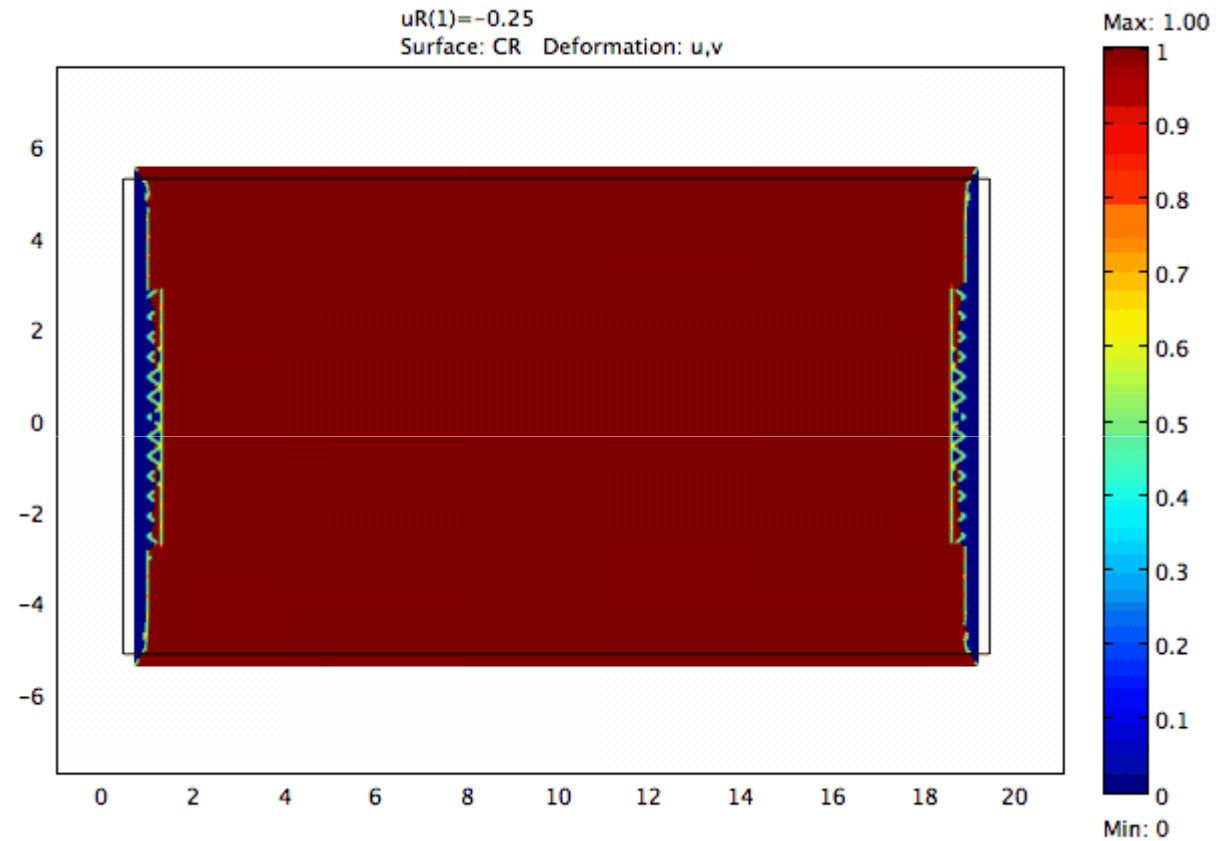


X-ray scattering (Zubarev et al.)

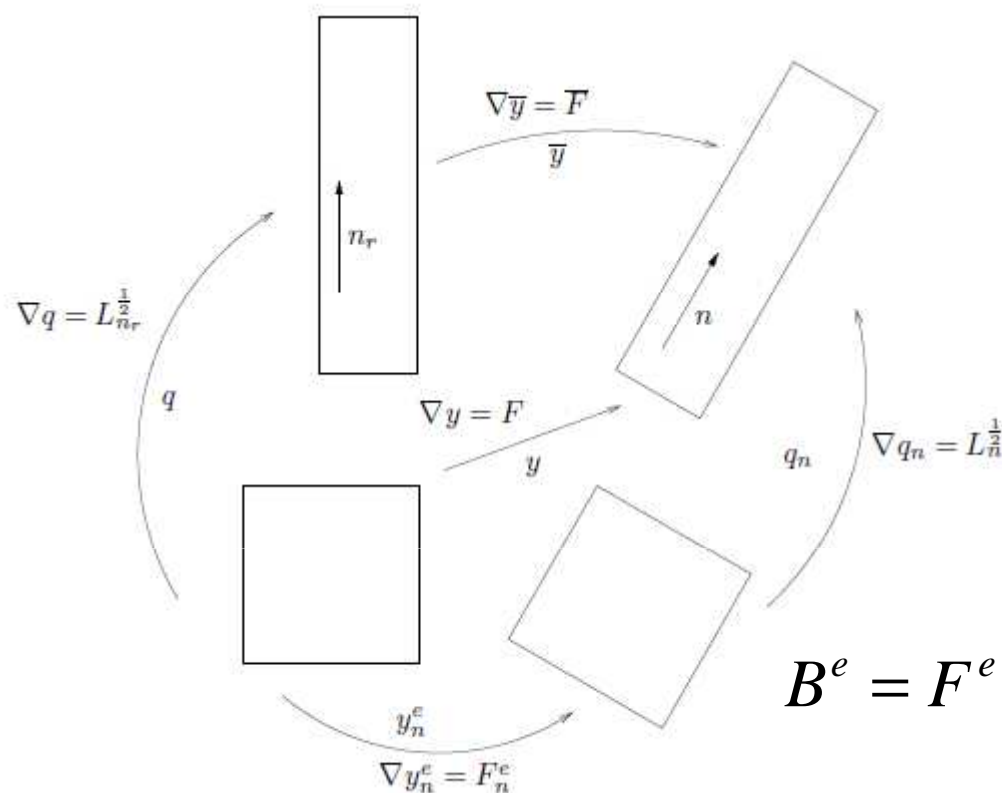


Direct observation (Terentjev)

Numerics with small strain theory



Large strains



$$F = L_n^{1/2} F^e$$

$$F^e = L_n^{-1/2} F$$

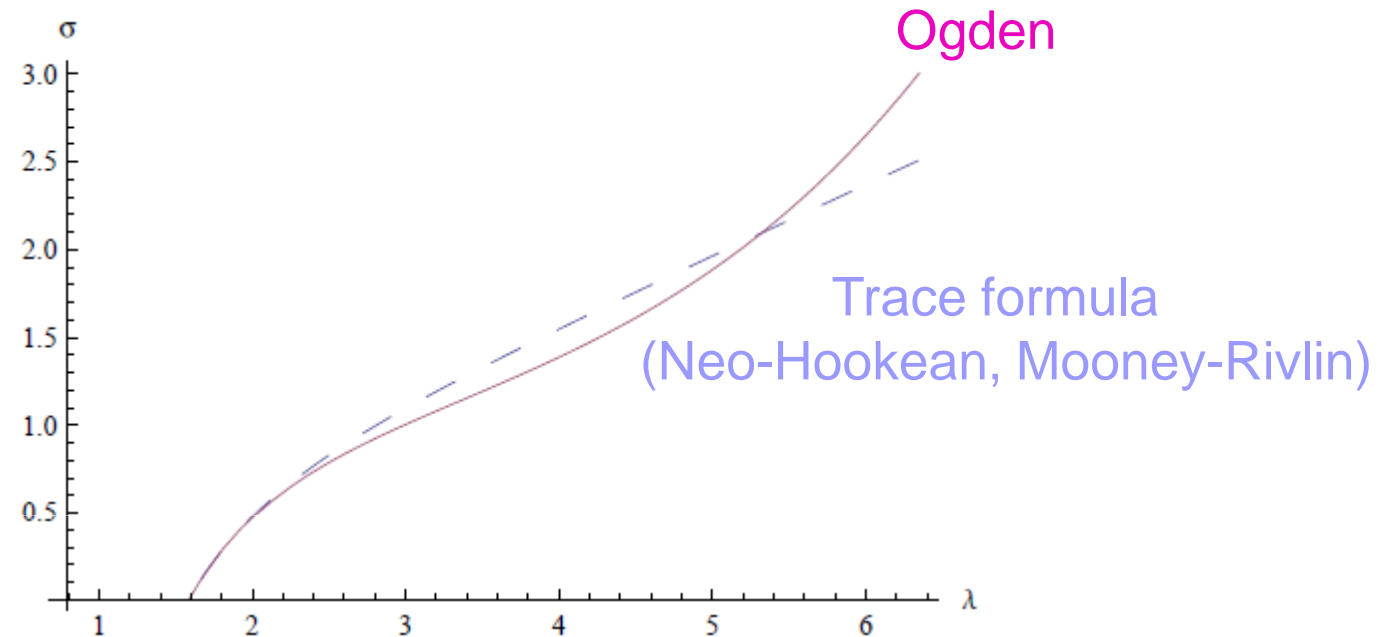
$$B^e = F^e (F^e)^T = L_n^{-1/2} F F^T L_n^{-1/2}$$

Ogden-type energy

$$\frac{\mu}{2} \text{Tr} B^e = \frac{\mu}{2} F F^T L_n^{-1} \cdot I = \sum_{i=1}^3 \frac{\mu}{2} \lambda_i (B^e)$$

$$\sum_{j=1}^K \sum_{i=1}^3 \frac{c_j}{\gamma_j} \lambda_i^{\gamma_j/2} (B^e)$$

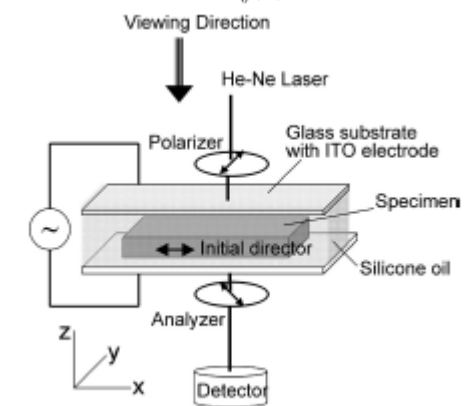
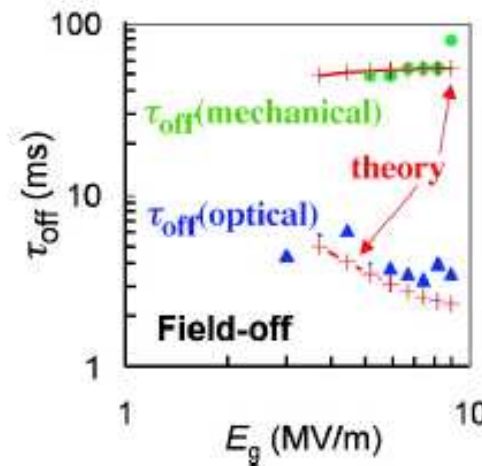
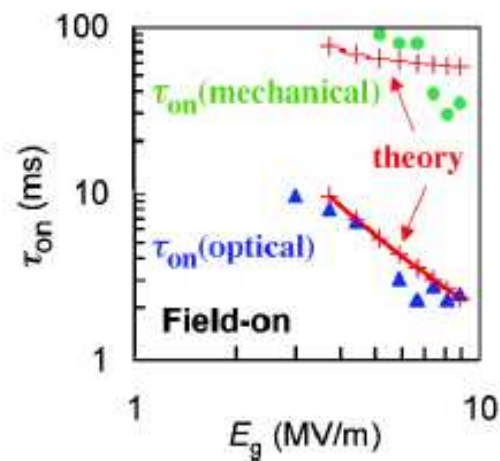
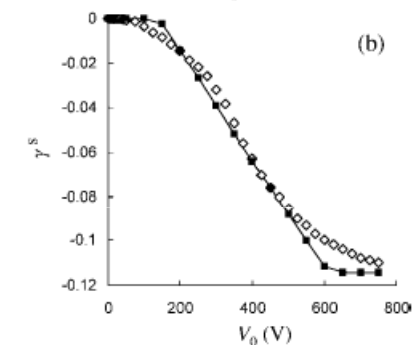
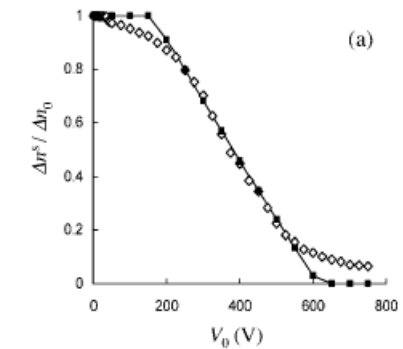
Ogden-type energies



Ogden: $c_1 = 1.5 \mu$, $\gamma_1 = 1.5$; $c_2 = 0.001 \mu$, $\gamma_2 = 5$;

Trace formula: $c_1 = \mu = 1$, $\gamma_1 = 2$.

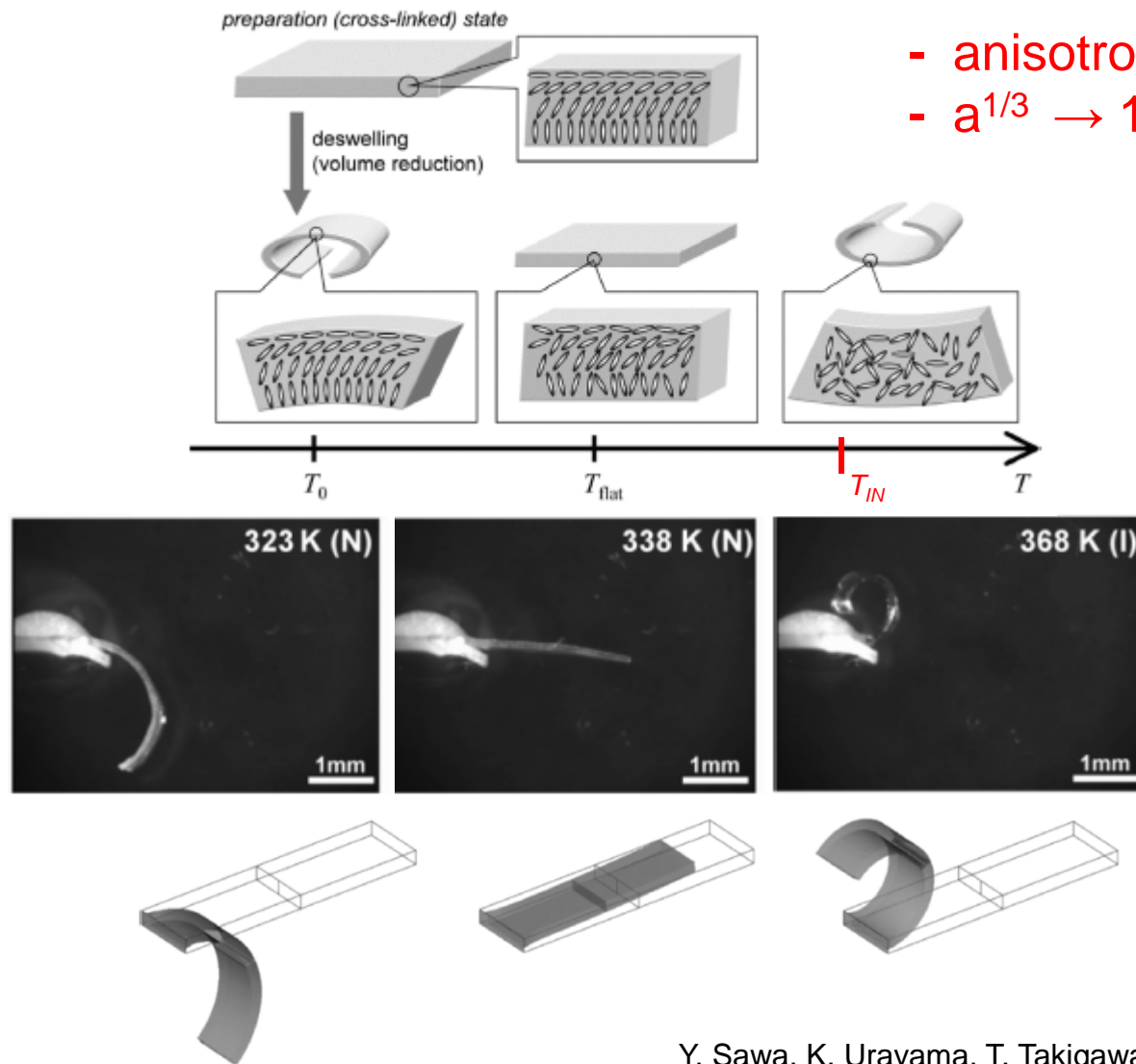
Response times of a contractile soft actuator (artificial muscles ?)



A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi:

[Dynamics of electro-opto-mechanical effects in swollen nematic elastomers](#), *Macromolecules*, vol.41, p. 9389 (2008).

Patterned nematic texture (soft manipulator)



- anisotropic swelling
- $a^{1/3} \rightarrow 1$ as $T \rightarrow T_{IN}$

Y. Sawa, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi:
Thermally driven giant bending of LCE films with hybrid alignment, *Macromolecules*, vol.43, p. 4362 (2010).

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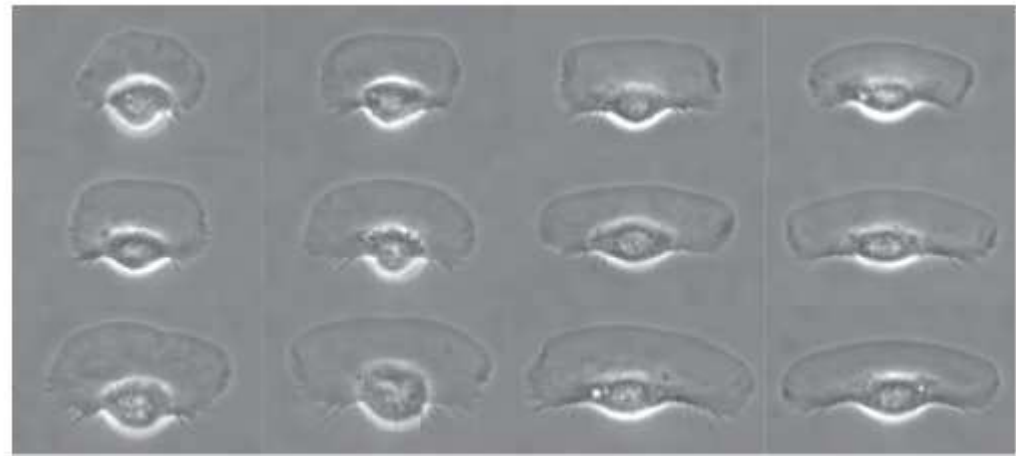
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Many contributions by many other authors.....

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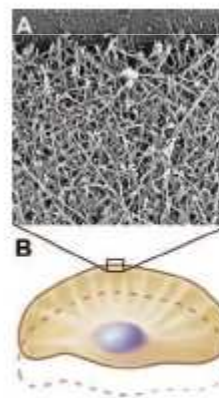
Cell motility and Biological Self-propulsion



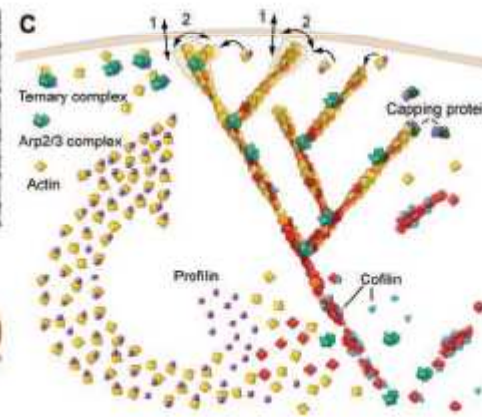
K. Keren et al. (2008)



Eutrep2.mov



T. D. Pollard and J. Berro (2009)



1) Protrusion of the Leading Edge



2) Adhesion at the Leading Edge



Deadhesion at the Trailing Edge



3) Movement of the Cell Body



R. Ananthakrishnan and A. Ehrlicher (2003)

keratocyte2.flv

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