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

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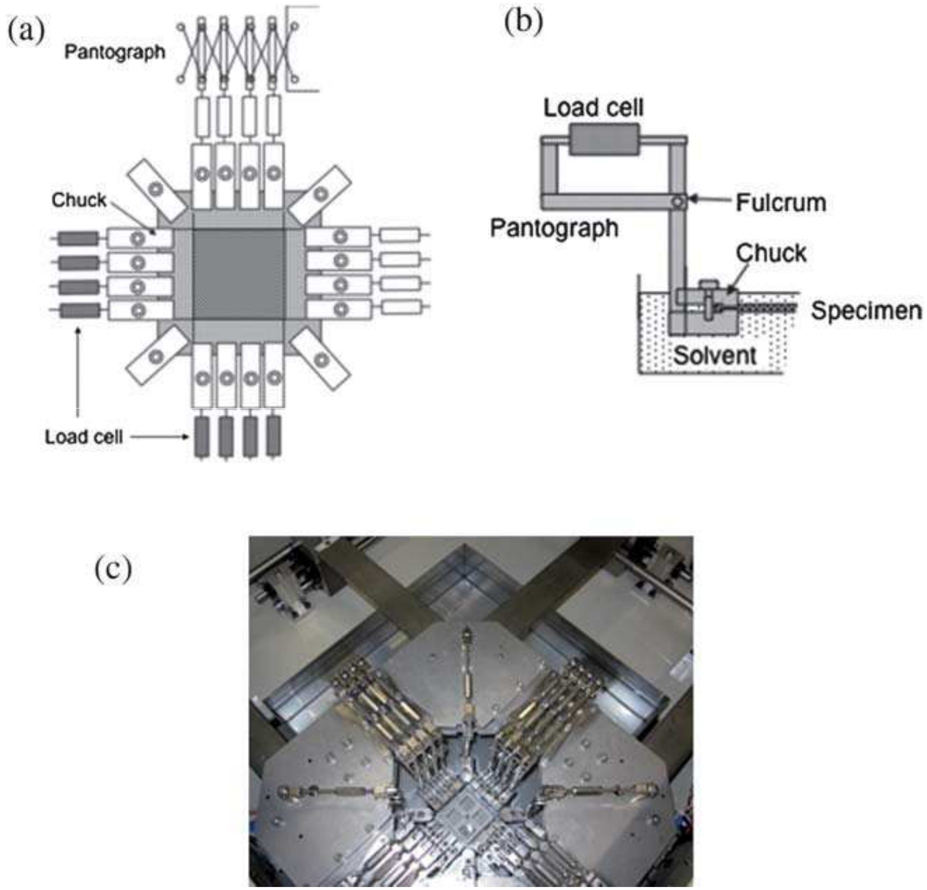
Biaxial stretching experiments on soft sheets

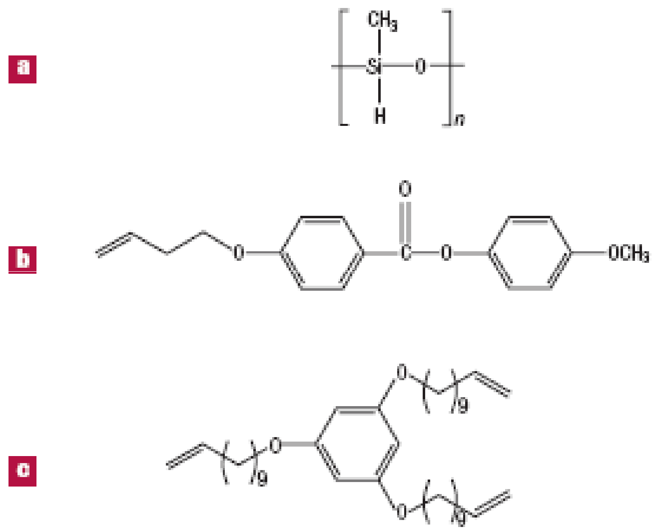


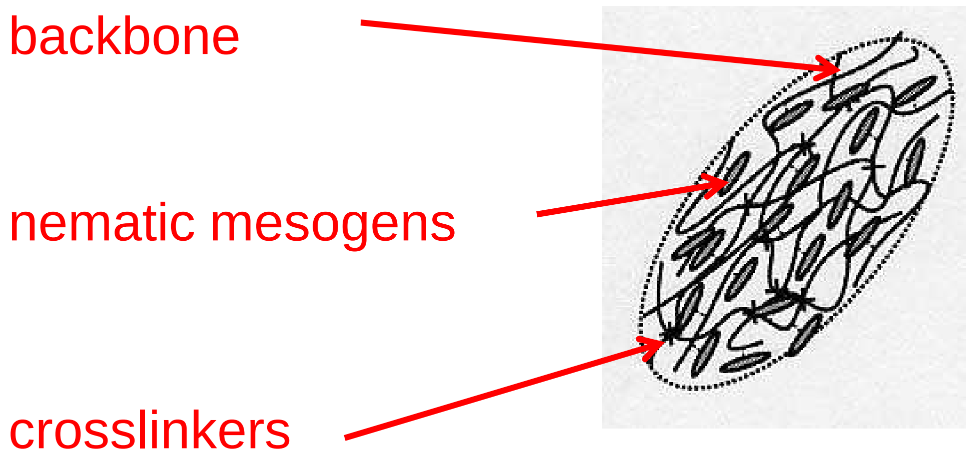
Urayama_c0sm00955e.mov

(K. Urayama)

What are Nematic Elastomers?

Cross-linked networks of polymeric chains containing nematic mesogens

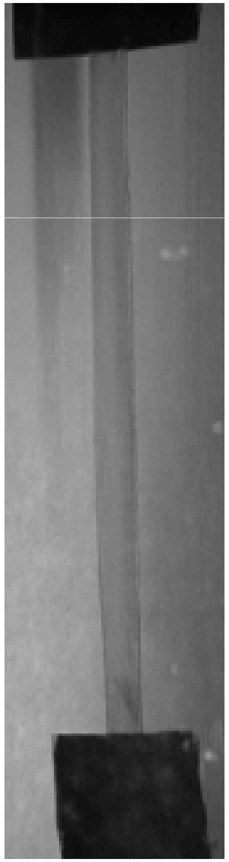




They combine optical properties and orientational DOFs typical of nematic LCs
(Frank curvature elasticity, dielectric anisotropy)
with translational DOFs of an elastic solid
(rubber elasticity)

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

Cross-linked networks of polymeric chains containing nematic mesogens:
alignment of mesogens along average direction **n**
induces spontaneous distortion of chains



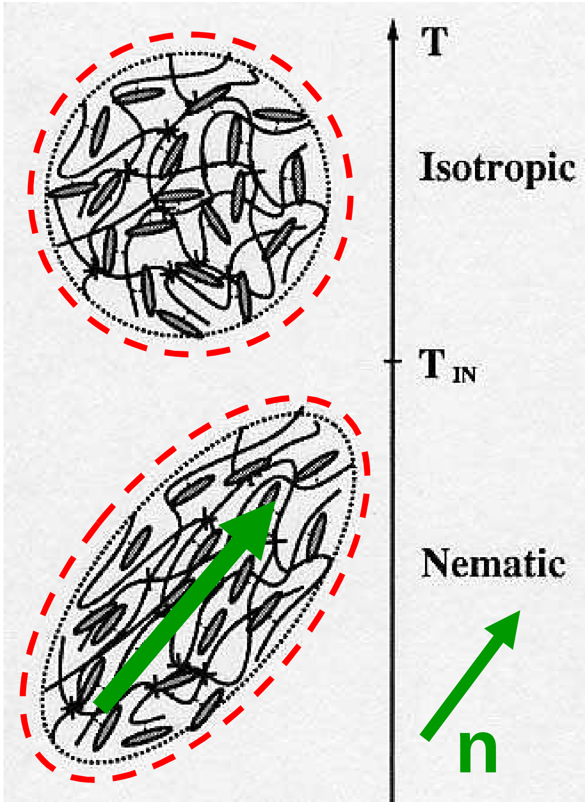
(H. Finkelmann)

Spontaneous distortion :

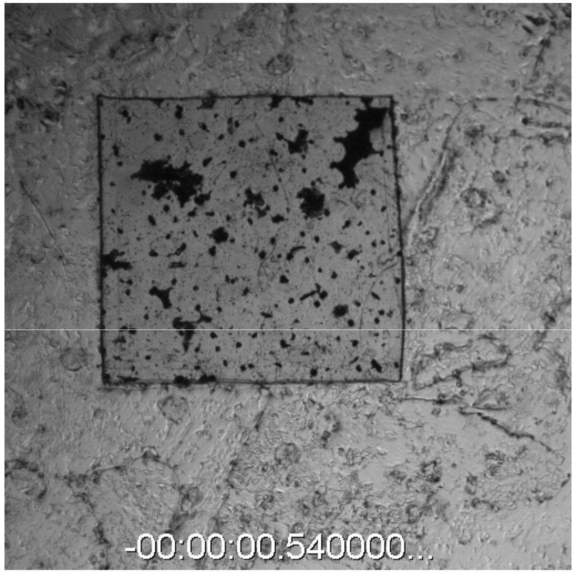
$$F_n = a^{1/3}\, n \otimes n + a^{-1/6}(I - n \otimes n)$$

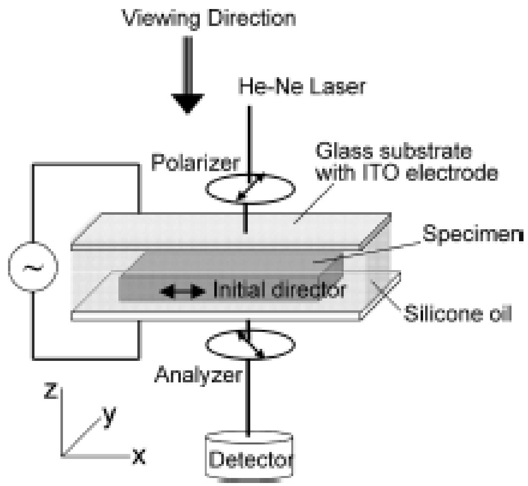
a volume preserving uniaxial extension along **n** of magnitude $a^{1/3} \geq 1 \quad (a > 1)$

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



Apply electric field to turn nematic director and spontaneous distortion

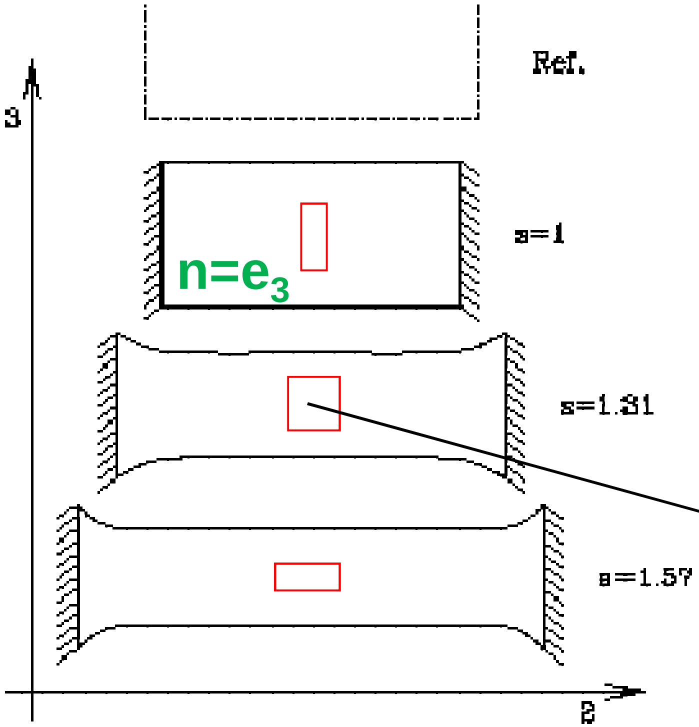


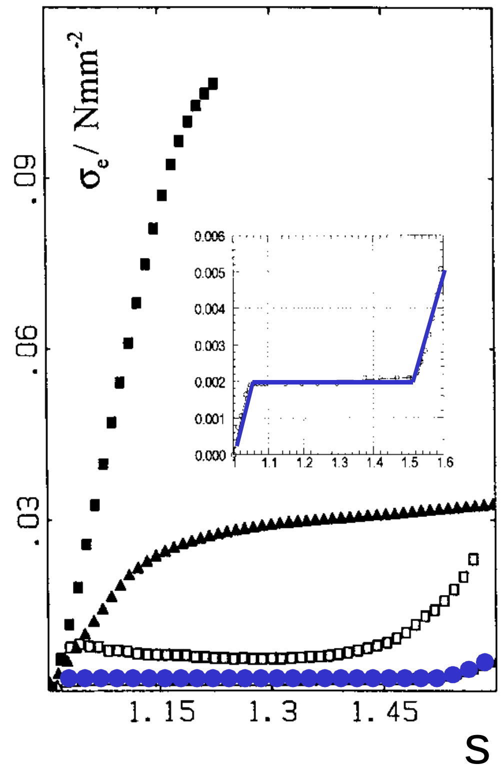


Purely mechanical stretching

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)



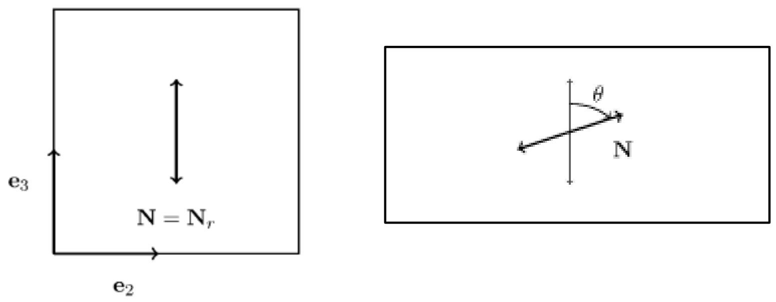


(H. Finkelmann, 95)

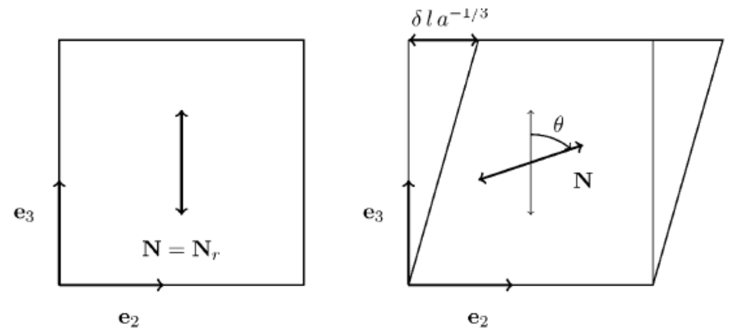
2: non-uniform director reorientation (stripe-domain instability)

Explore energy landscape through homogeneous stretch and shear: instabilities

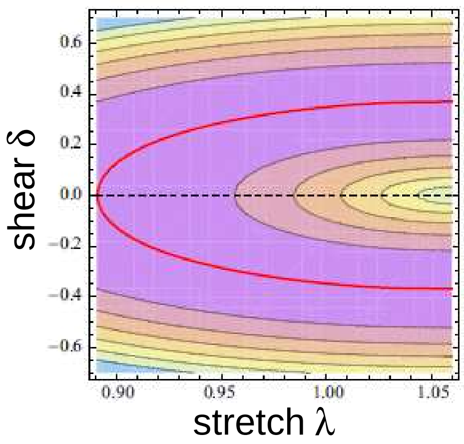
Stretch by λ

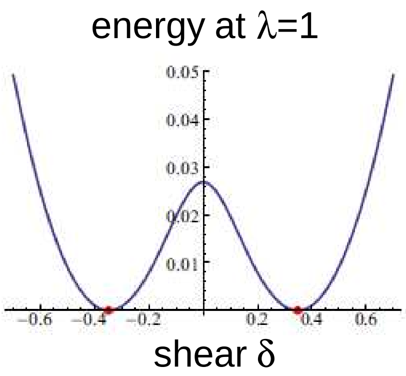


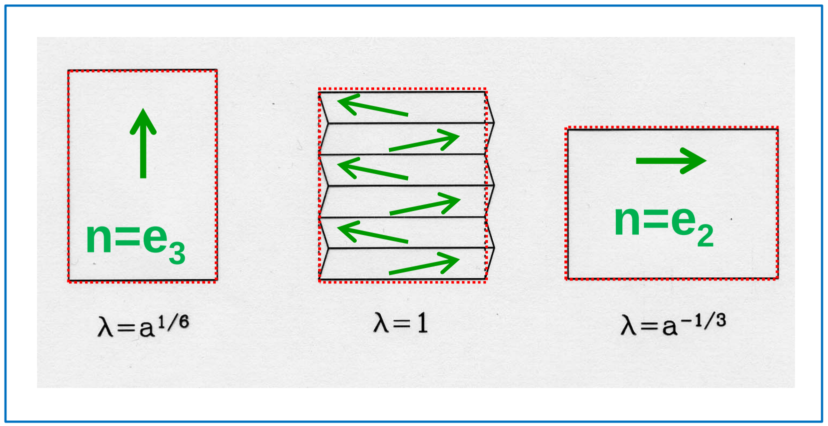
Shear by δ



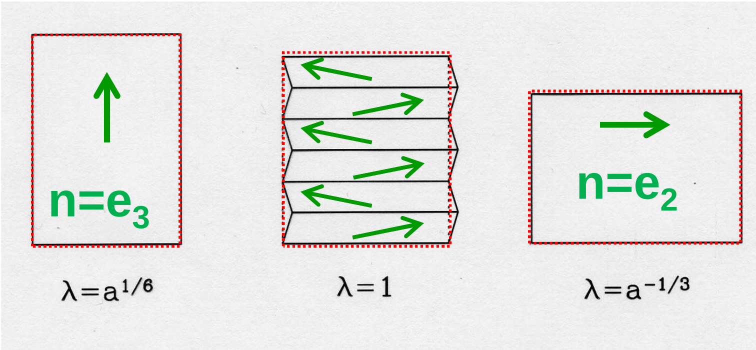
$\min_n W(F,n)$ (isotropic)



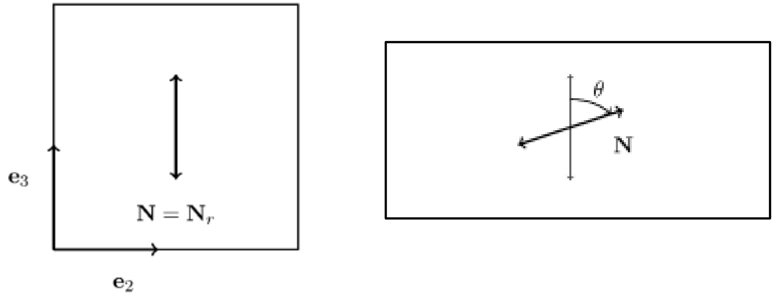




Similar instabilities for anisotropic energy

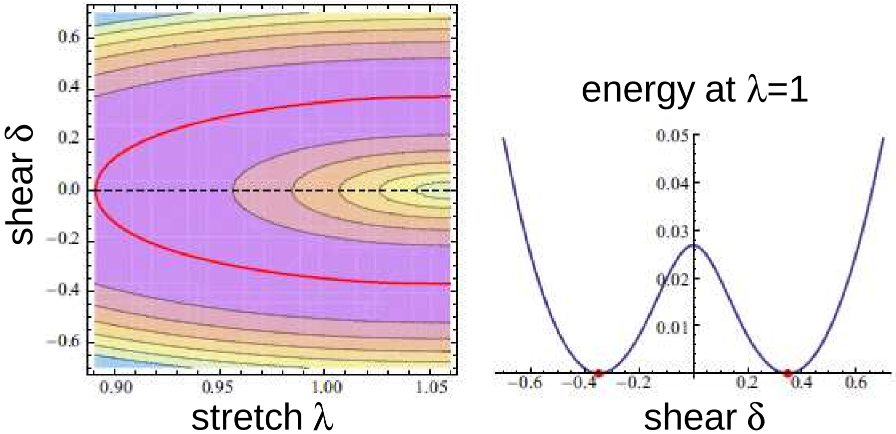


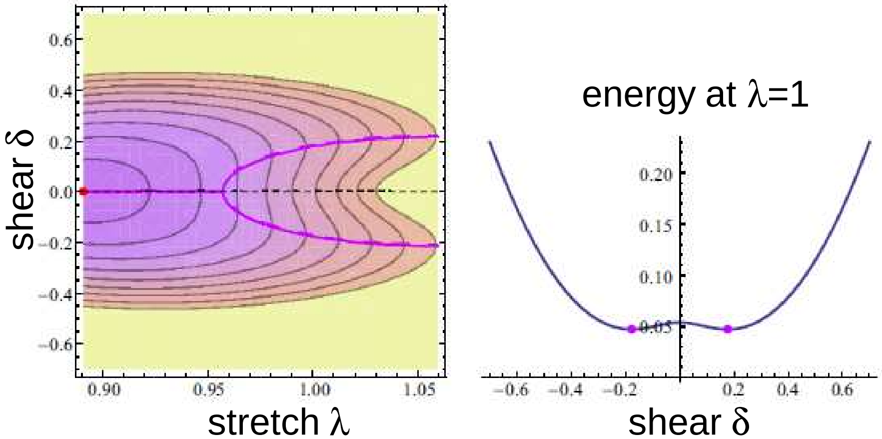
Stretch by λ



$\min_n W(F,n)$ (isotropic)

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





Can use small strain theory as well

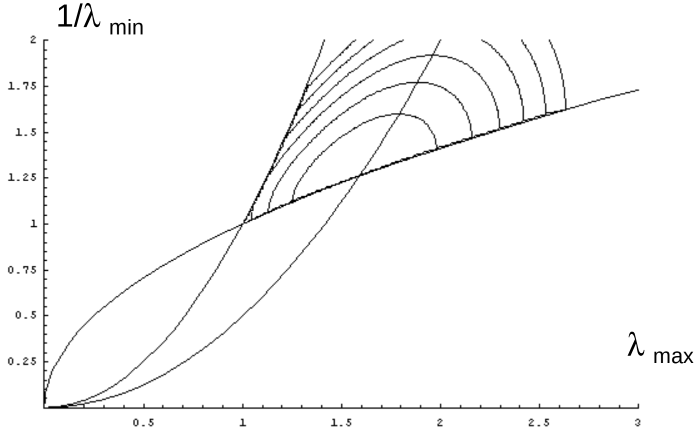
$a^{1/3} = 1 + \gamma\,, \;\; \gamma << 1$

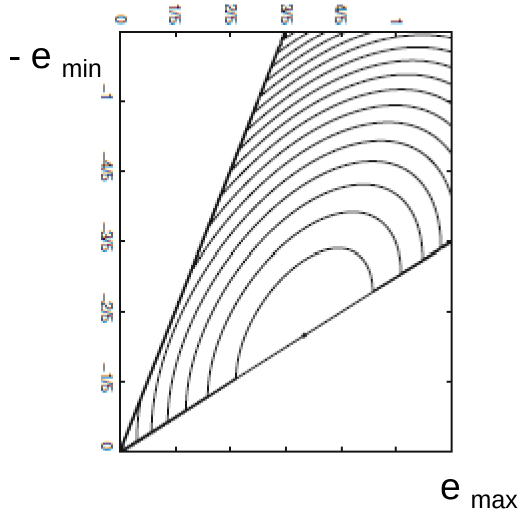
measures spontaneous stretch along n

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

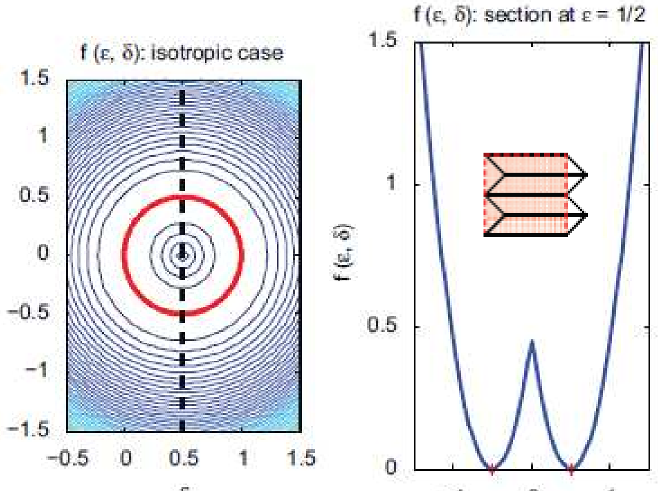
$E_0(n) = 3/2\, \gamma\, (n \otimes n - 1/3\, I\,)$

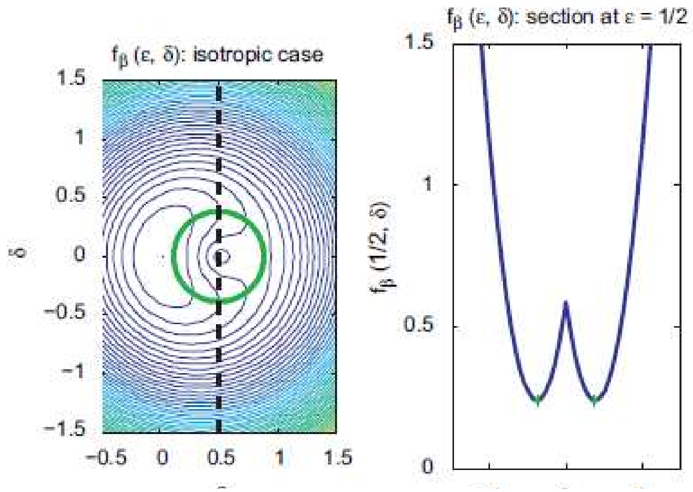
$W(F,n) = ½\, \mu\, (F F^T) \bullet (F_n F_n^T)^{-1} \longrightarrow \mu\, |\, E - E_0(n)\, |^2$



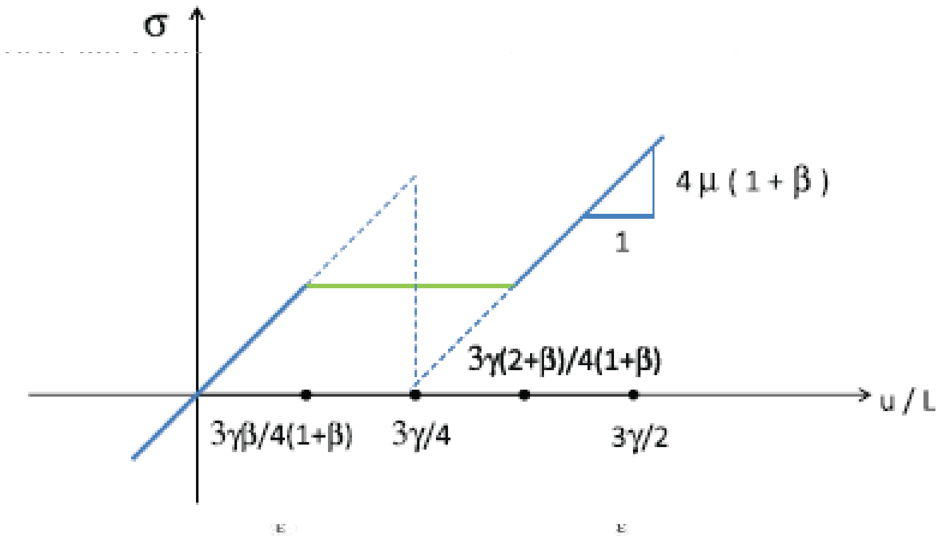


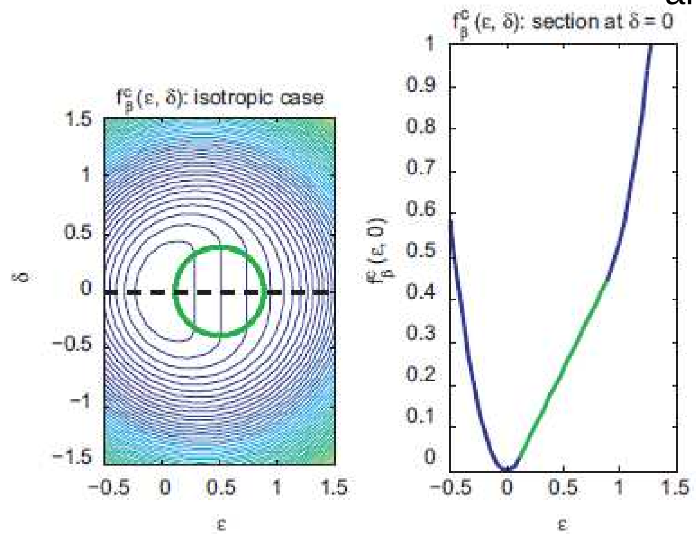
QC envelopes (plane strain, extension-shear)



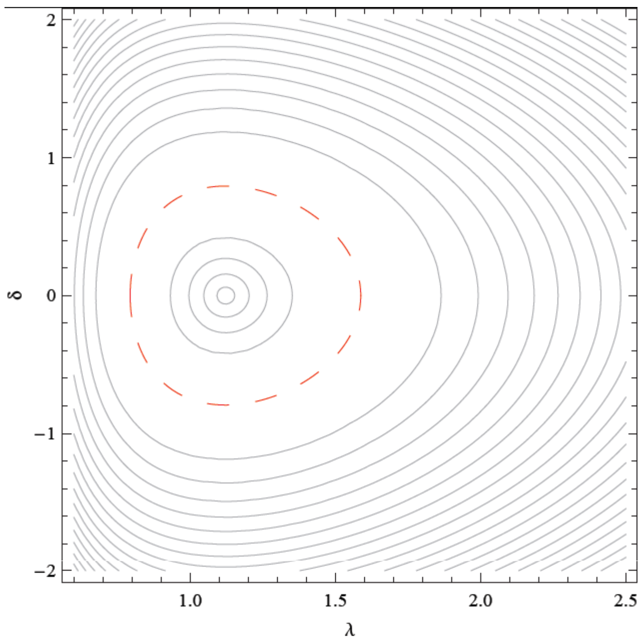


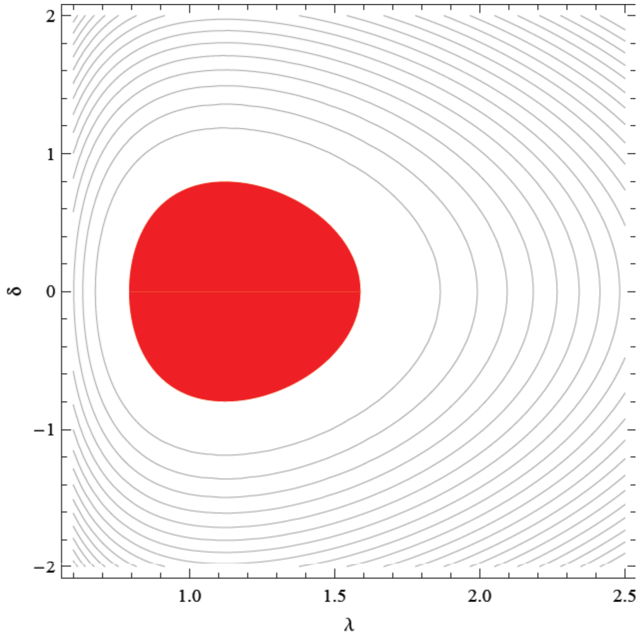
anisotropic

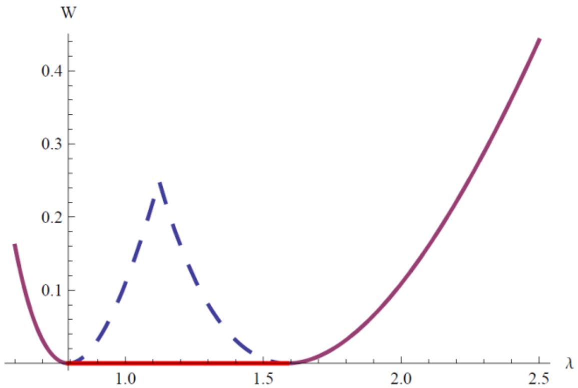


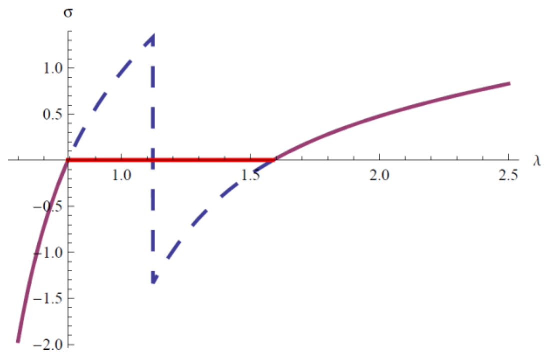


Finite elasticity (isotropic, plane strain)

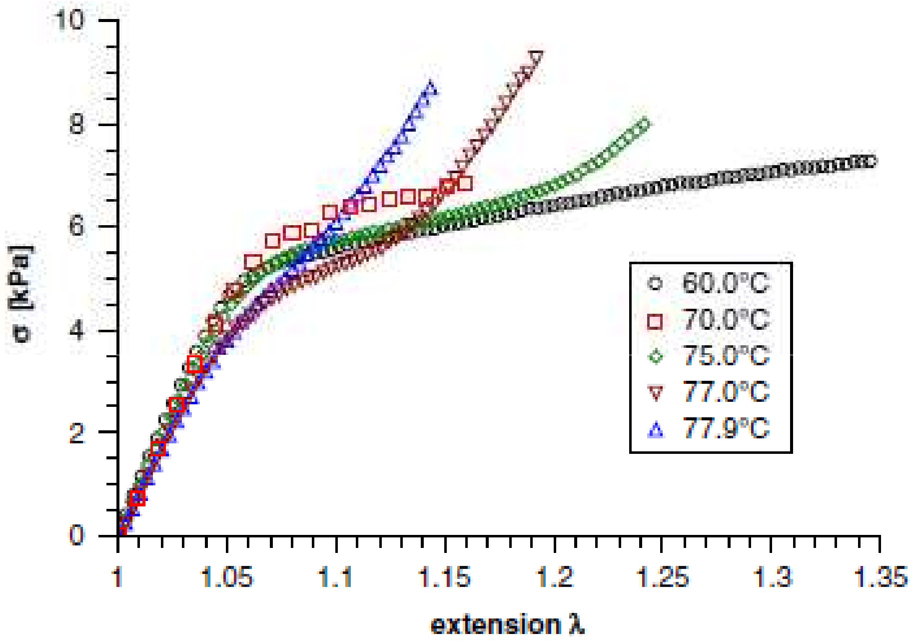


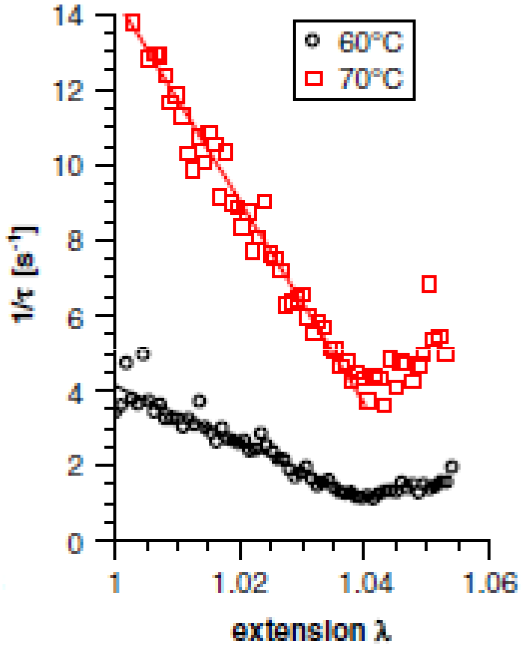






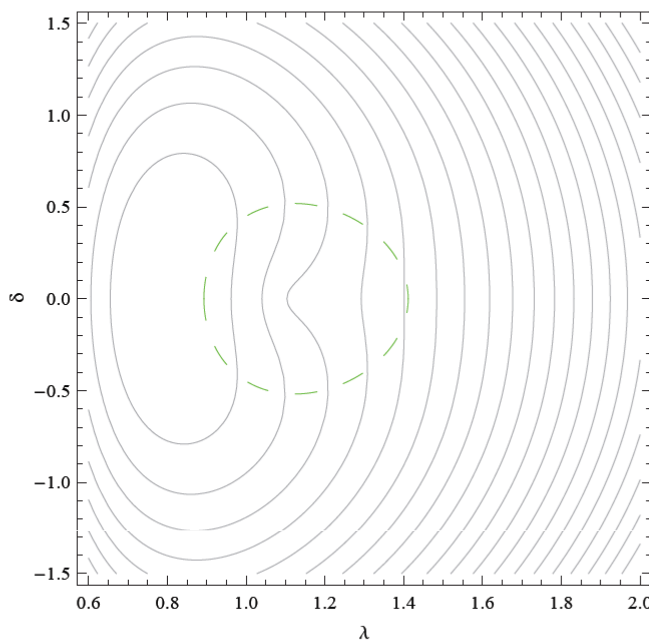
Soft response to stretch and vanishing of shear modulus after threshold stretch

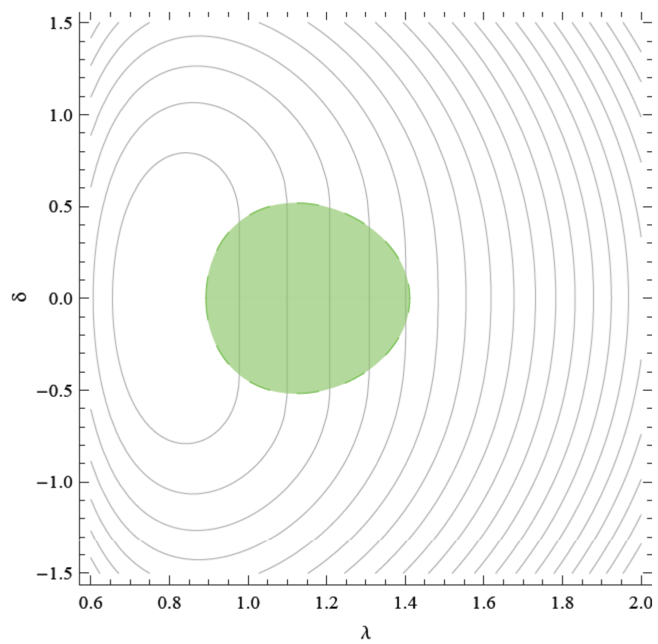


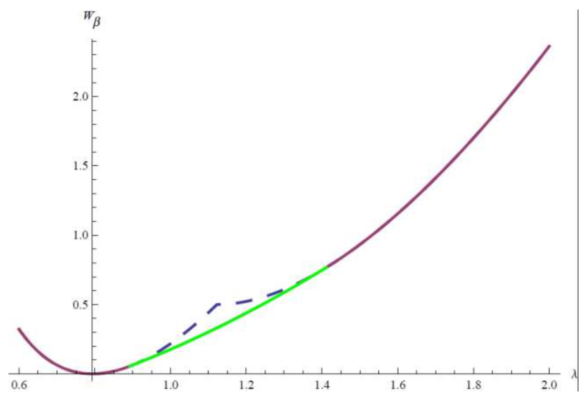


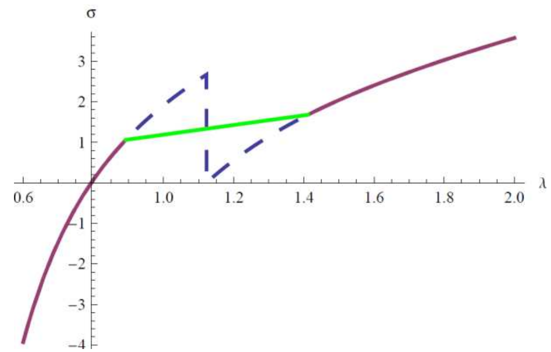
(M. Copic)

Finite elasticity (anisotropic, plane strain)

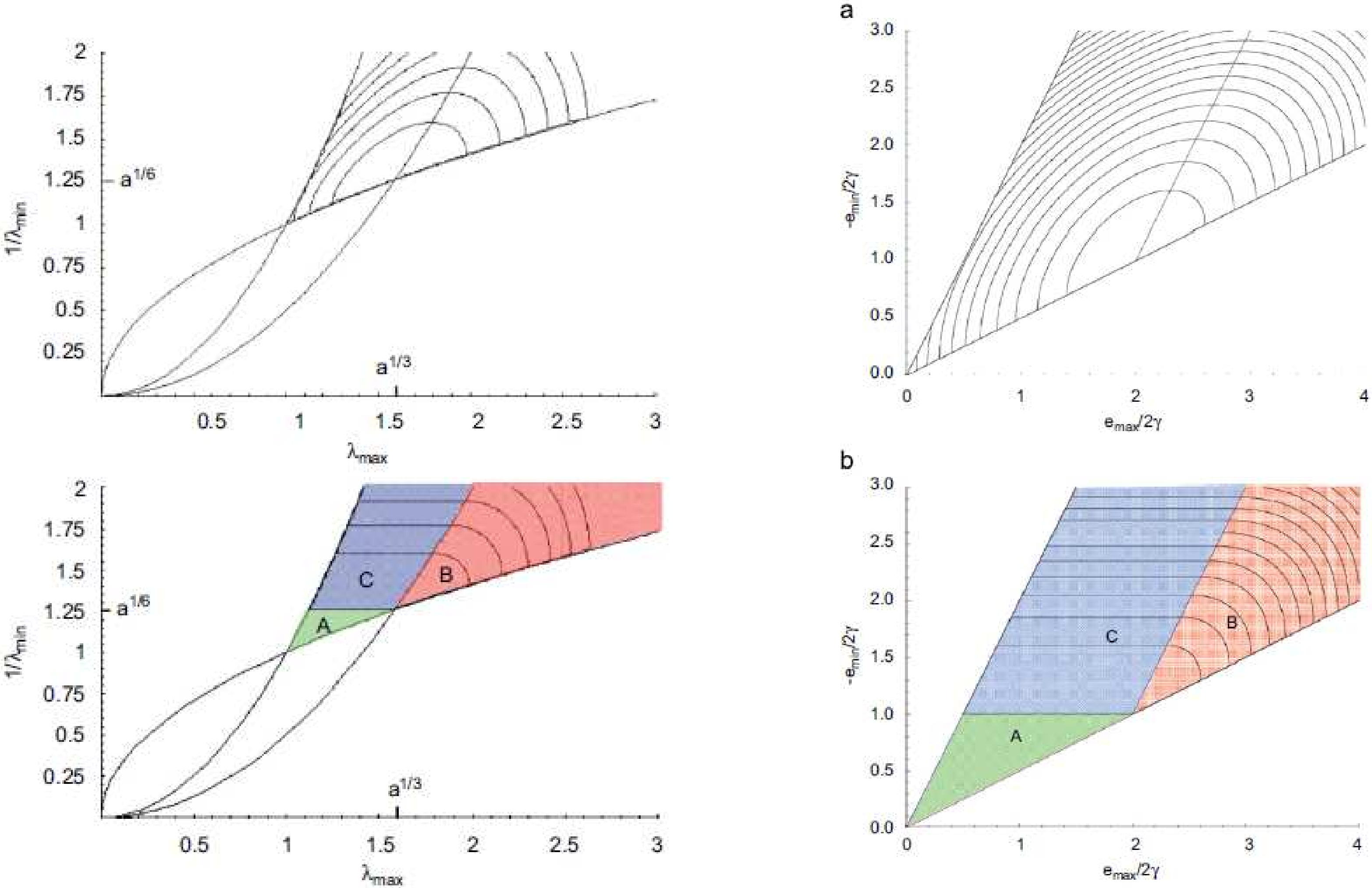








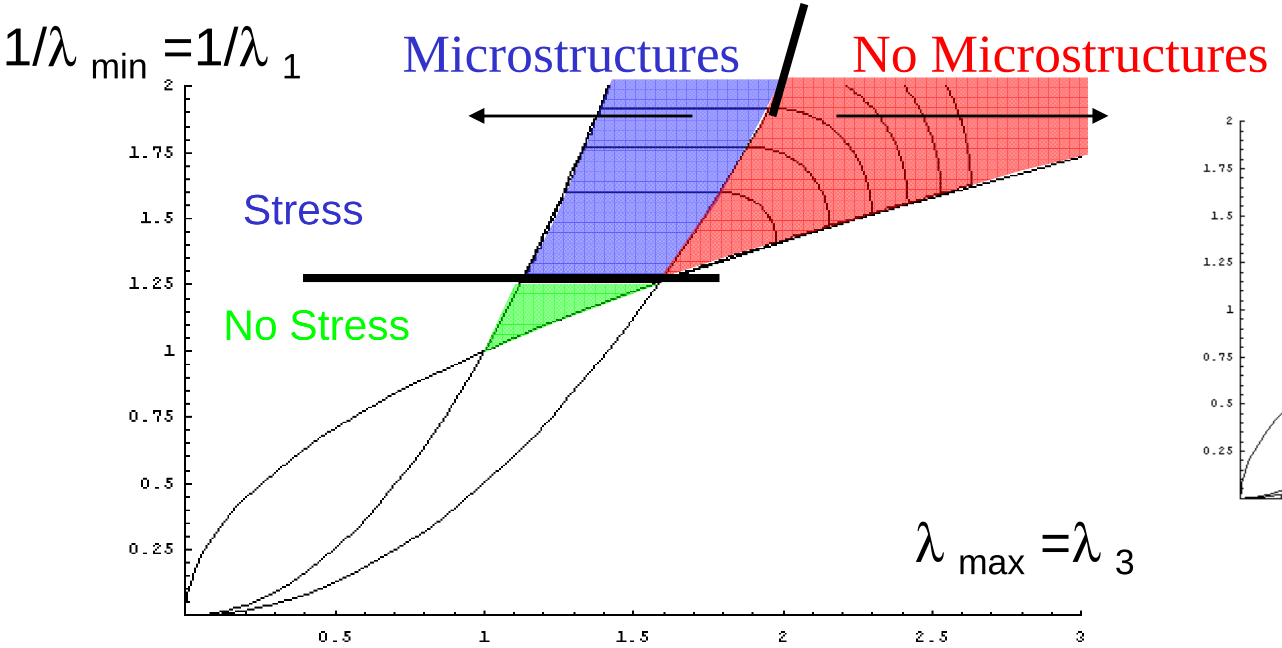
QC envelopes (3d, isotropic)

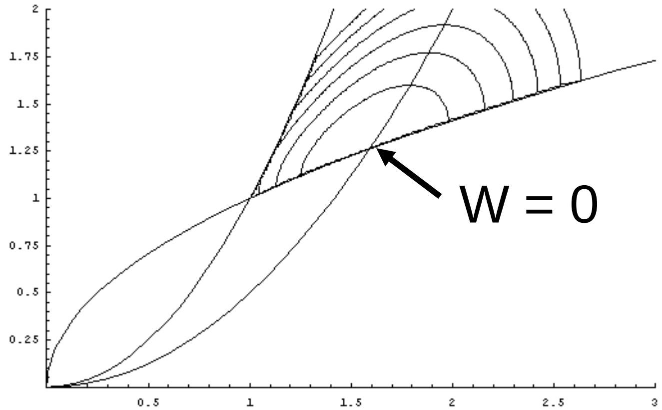


The quasi-convexified energy W^{qc}

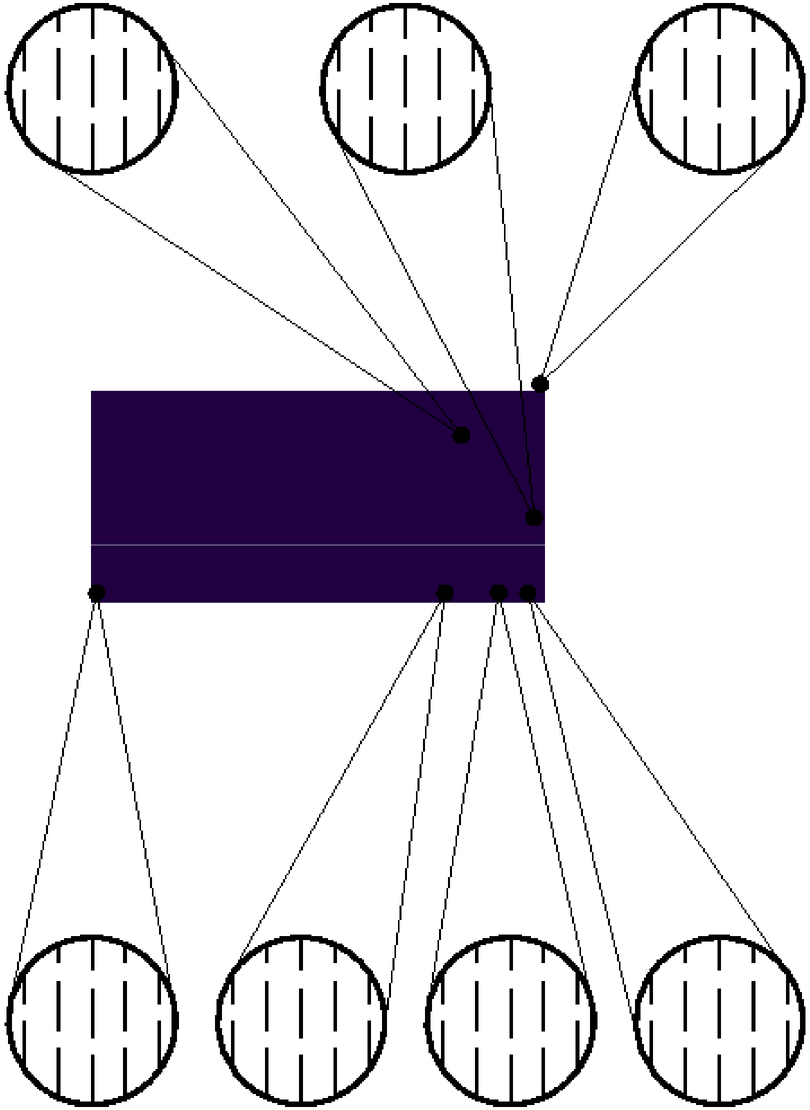
$$W^{qc}(F) = \begin{cases} 0 & \text{(phase L) if } \lambda_1 \geq a^{1/6} \\ W(F) & \text{(phase S) if } a^{1/2}\lambda_3^2\lambda_1 > 1 \\ \lambda_1^2 + 2a^{1/2}\lambda_1^{-1} - 3a^{1/3} & \text{(phase I or Sm) else} \end{cases}$$

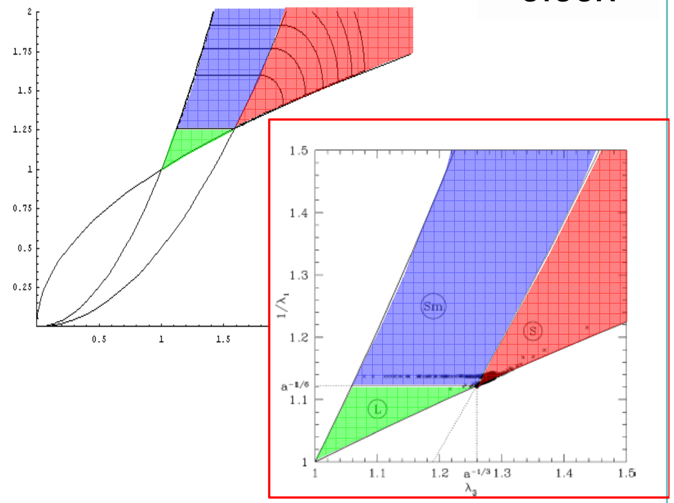
if $\det F = 1$, $W^{qc}(F) = +\infty$ if $\det F \neq 1$.

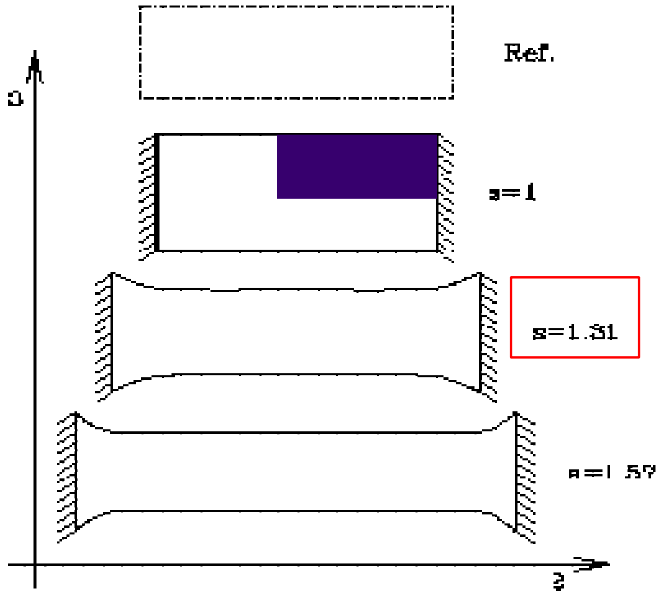




Use W^{qc} in numerical stretching experiment

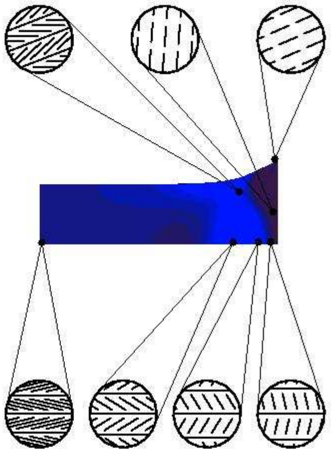


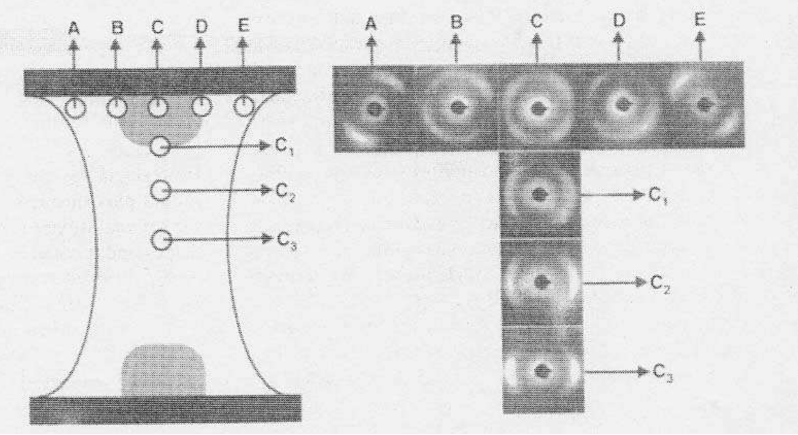




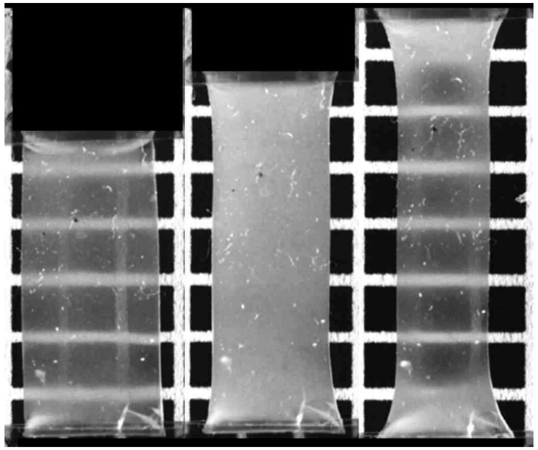
Theory vs. Experiment

Multiscale numerics



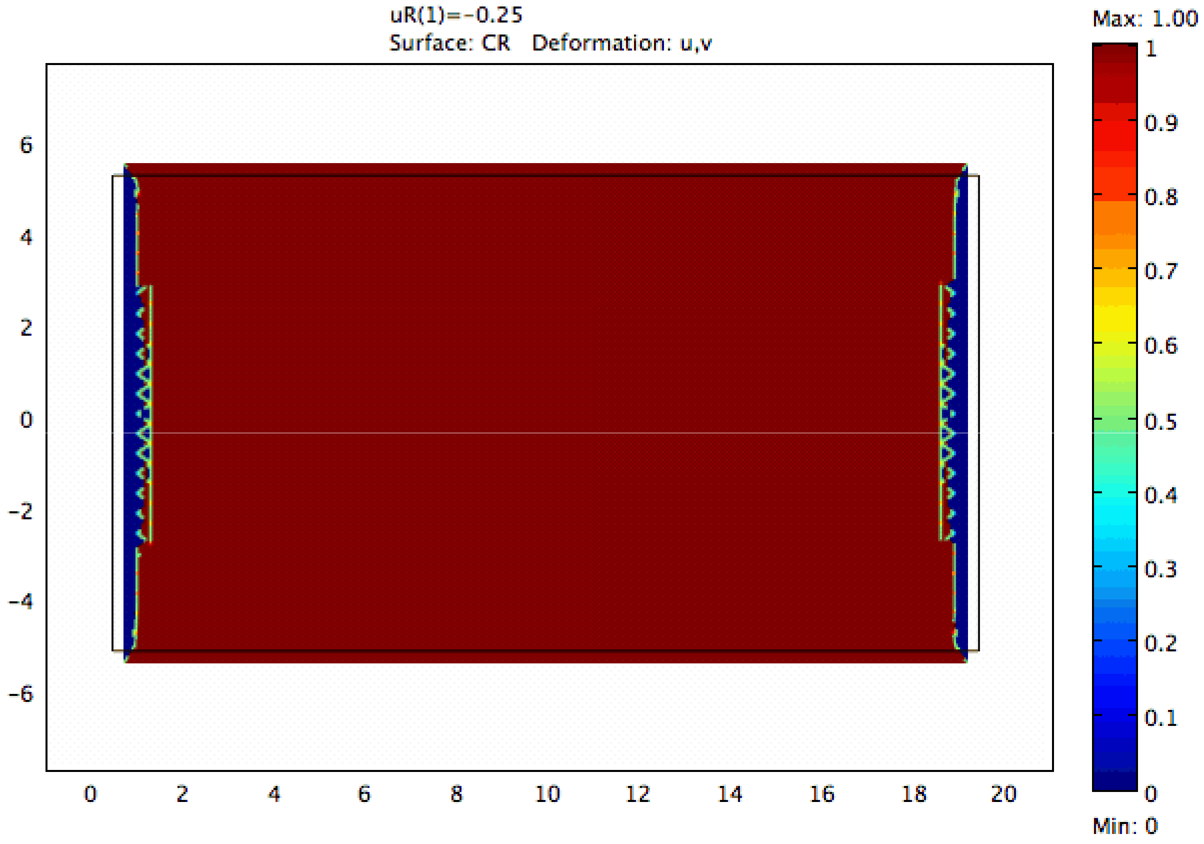


X-ray scattering (Zubarev et al.)

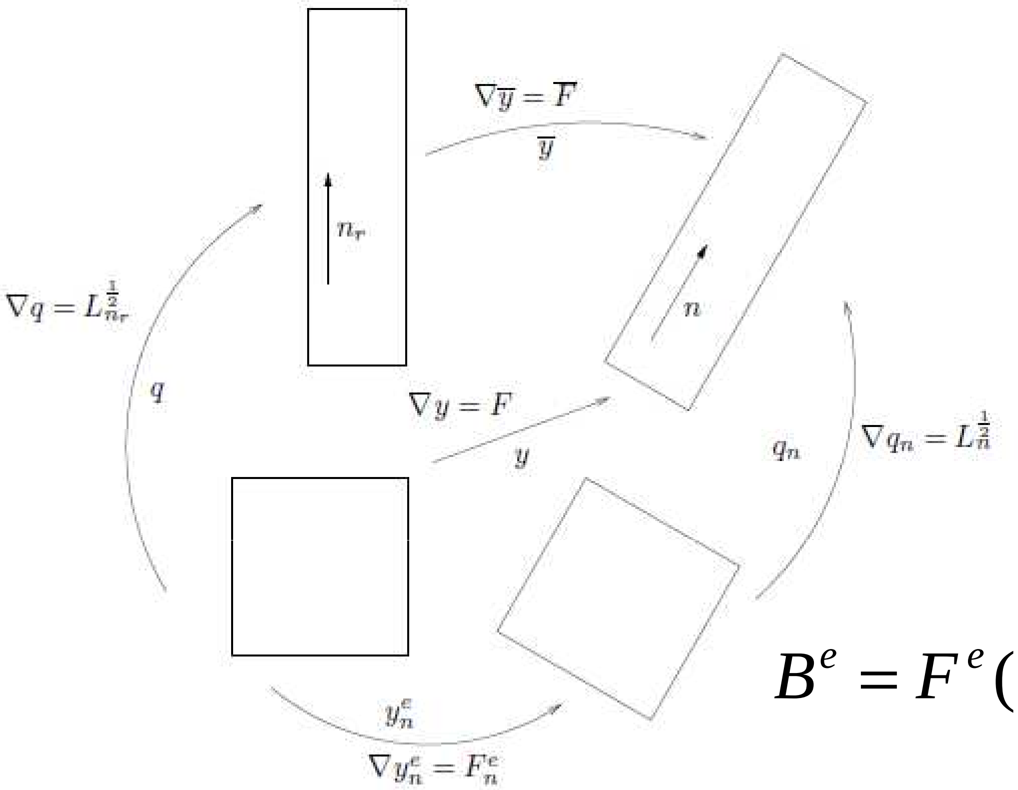


Direct observation (Terentjev)

Numerics with small strain theory



Large strains



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

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

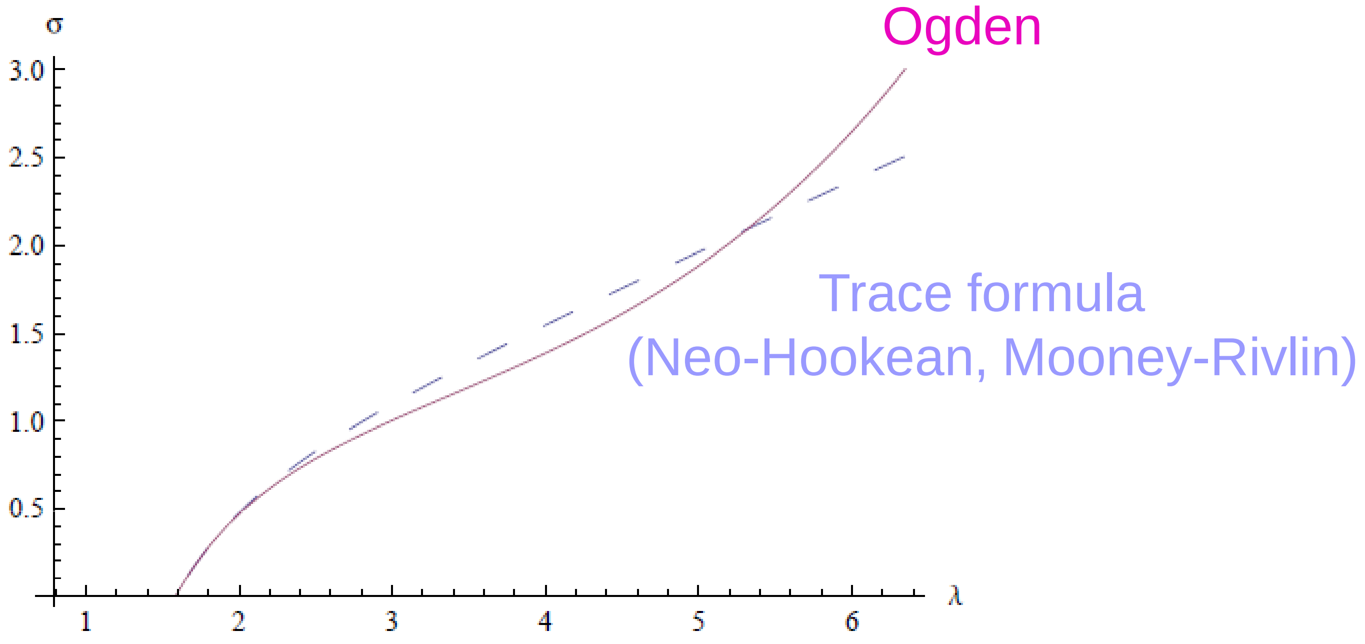
$$B^e = F^e (F^e)^T = L_n^{-1/2} F F^T L_n^{-1/2}$$

Ogden-type energy

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

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

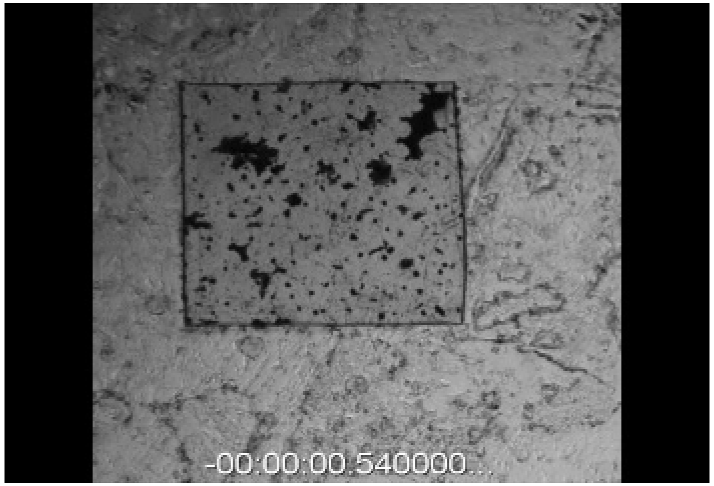
Ogden-type energies

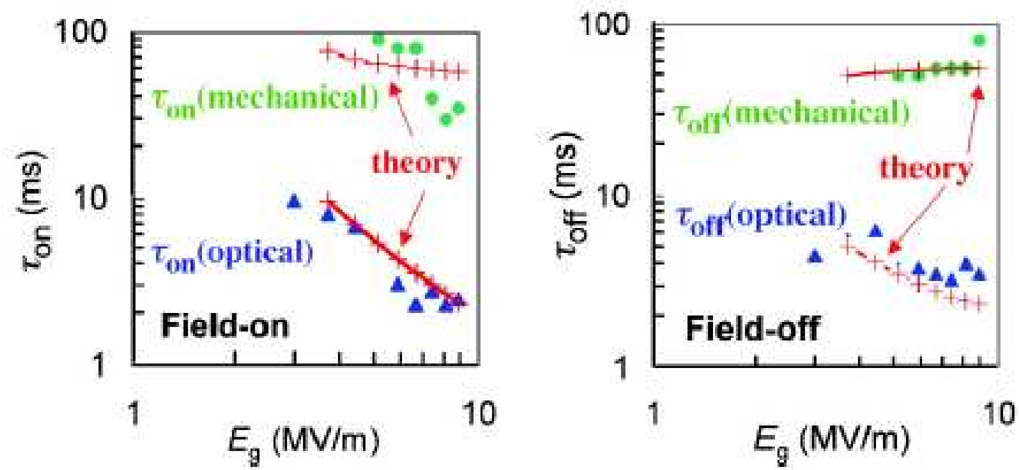


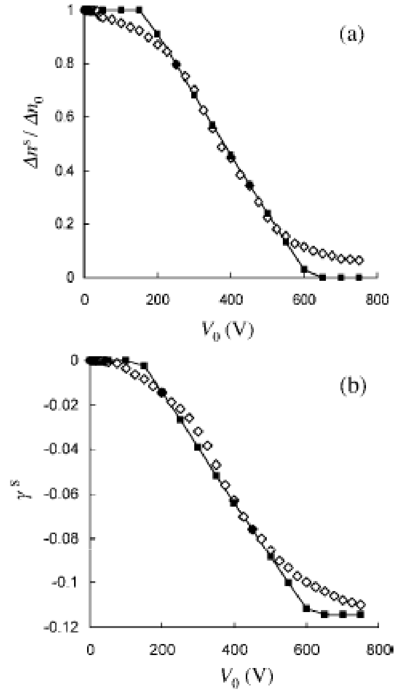
Ogden: $c_1 = 1.5\,\mu$, $\gamma_1 = 1.5$; $c_2 = 0.001\,\mu$, $\gamma_2 = 5$;

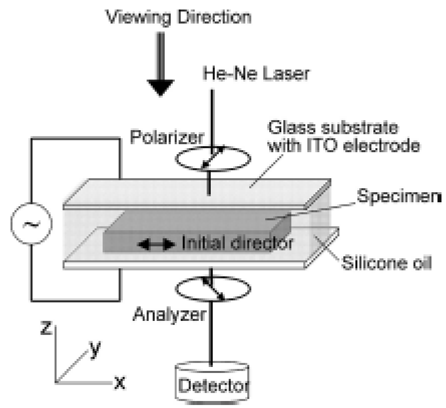
Trace formula: $c_1 = \mu = 1$, $\gamma_1 = 2$.

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





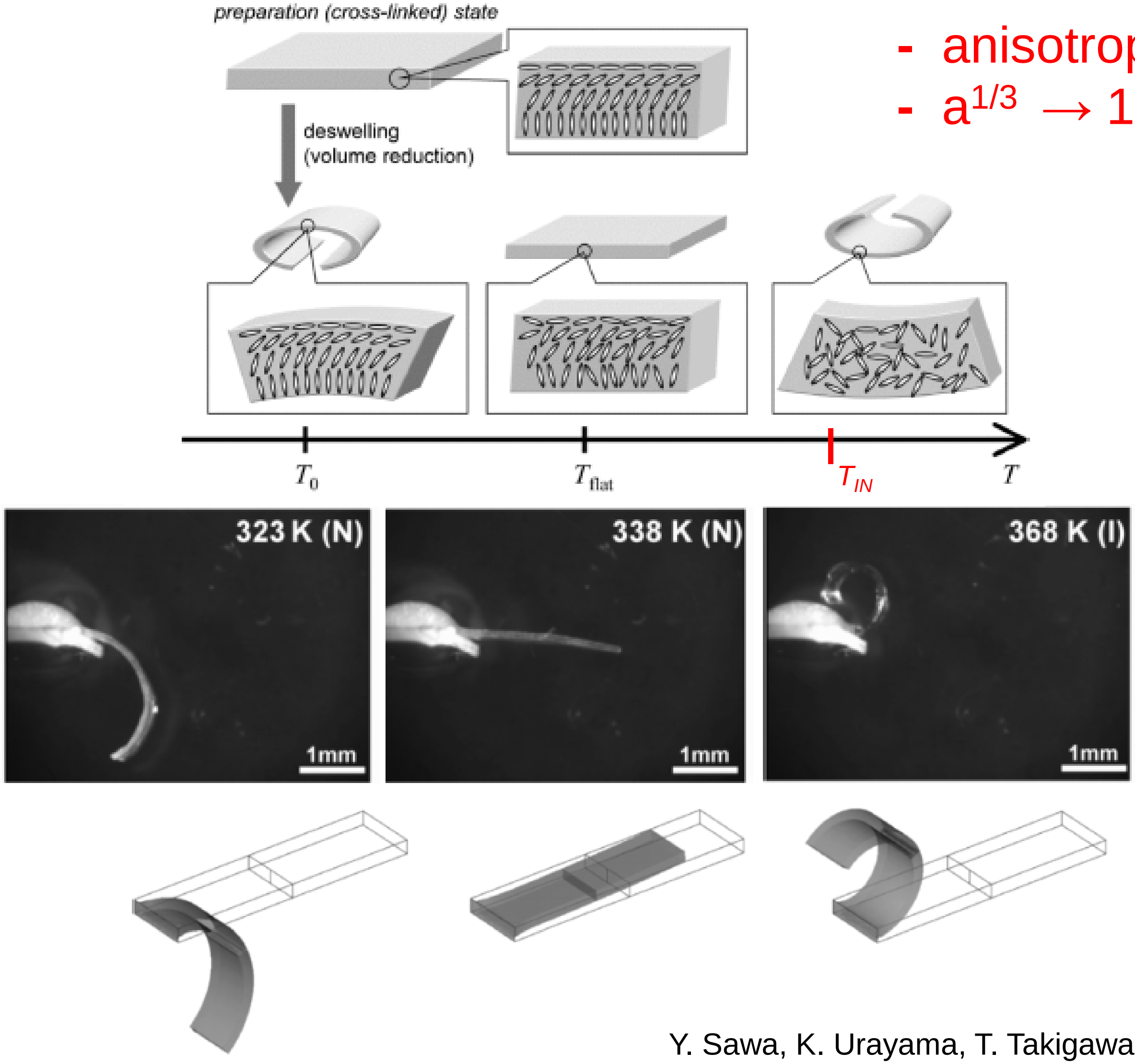




A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi:
Dynamics of electro-opto-mechanical effects in swollen nematic elastomers, Macromolecules, vol.41, p. 9389 (2008).

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).

References

- A. DeSimone, *Energetics of fine domain structures*, Ferroelectrics, vol. 222, p. 275 (1999).
- A. DeSimone and G. Dolzmann, *Material instabilities in nematic elastomers*, Physica D, vol. 136, p. 175 (2000).
- A. DeSimone and G. Dolzmann, *Macroscopic response of nematic elastomers via relaxation of a class of SO(3)-invariant energies*, Archive Rat. Mech. Analysis, vol. 161, p. 181 (2002).
- S. Conti, A. DeSimone, and G. Dolzmann, *Soft elastic response of stretched sheets of nematic elastomers: a numerical study*, J. Mech. Phys. Solids, vol. 50, p. 1431 (2002).
- S. Conti, A. DeSimone, and G. Dolzmann, *Semi-soft elasticity and director reorientation in stretched sheets of nematic elastomer*, Phys. Rev. E, vol. 60, p. 61710 (2002).
- A .DeSimone and G. Dolzmann, *Stripe-domains in nematic elastomers:old and new*, in: IMA Volumes in Mathematics and its Applications, Springer Verlag, 2005.
- J. Adams, S. Conti, and A. DeSimone, *Soft elasticity and microstructure in smectic C elastomers*, Cont. Mech. and Thermodynamics, vol.18, p.319 (2007).
- J. Adams, S. Conti, A. DeSimone, and G. Dolzmann, *Relaxation of some transversally isotropic energies and applications to smectic A elastomers*, Math Mod. Meth. Appl. Sci., vol. 18, p. 1 (2008).
- M. Cicalese, A. DeSimone, and C. Zeppieri: *Discrete-to-continuum limits for strain-alignment-coupled systems: magnetostrictive solids, ferroelectric crystals and nematic elastomers,* Networks and Heterogeneous Media, vol. 4, p. 267 (2009).

References continued

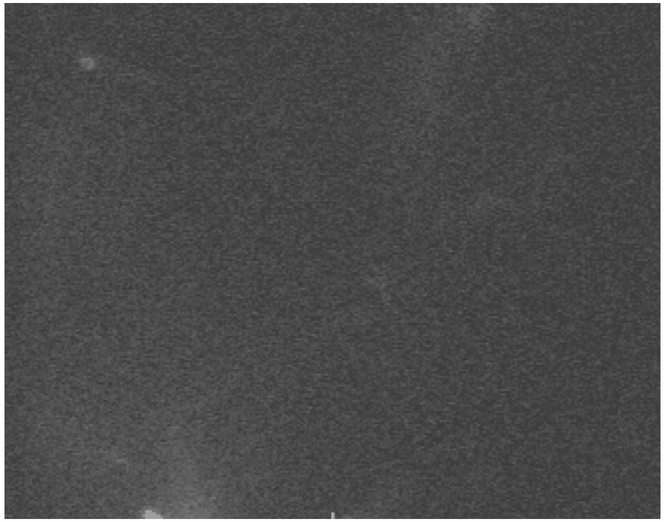
- A. DeSimone, A. DiCarlo, and L.Teresi, *Critical voltages and blocking stresses in nematic gels*, Eur. Phys. J. E, vol. 24, p. 303 (2007).
- A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, and L.Teresi, *Dynamics of electro-opto-mechanical effects in swollen nematic elastomers*, Macromolecules, vol.,41, p. 9389 (2008).
- A. DeSimone and L.Teresi, *Elastic energies for nematic elastomers*, Eur. Phys. J. E, vol. 29, p. 191 (2009).
- P. Cesana and A. DeSimone, *Strain-order coupling in nematic elastomers: equilibrium configurations*, Math. Meth. Mod. Appl. Sci., vol. 19, p. 601 (2009).
- Y. Sawa, K. Urayama, T. Takigawa, A. DeSimone, and L.Teresi, *Thermally driven giant bending of LCE films with hybrid alignment*, Macromolecules, vol.,43, p. 4362 (2010).
- P. Cesana, *Relaxation of multiwell energies in linearized elasticity and application to nematic elastomers*, Archive Rat. Mech. Analysis (2010).
- P. Cesana and A. DeSimone, *Quasiconvex envelopes of energies for nematic elastomers in the small strain regime and applications*, J. Mech. Phys. Solids, vol. 59, p. 787 (2011).
- V. Agostiniani, A. DeSimone, *Gamma-convergence of energies for nematic elastomers in the small strain limit*, Cont. Mech.Thermodynamics, vol. 23, p. 257 (2011).
- V. Agostiniani, A. DeSimone, *Ogden-type energies for nematic elastomers*, submitted (2011).

Many contributions by many other authors.....

Monograph:

M. Warner and E. Terentjev, *Liquid Crystal Elastomers,* Oxford University Press, 2003.

Cell motility and Biological Self-propulsion



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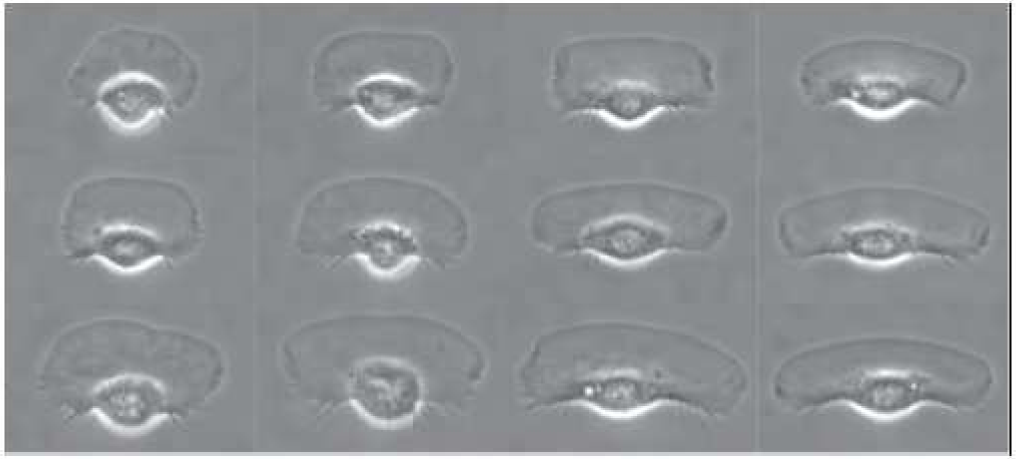
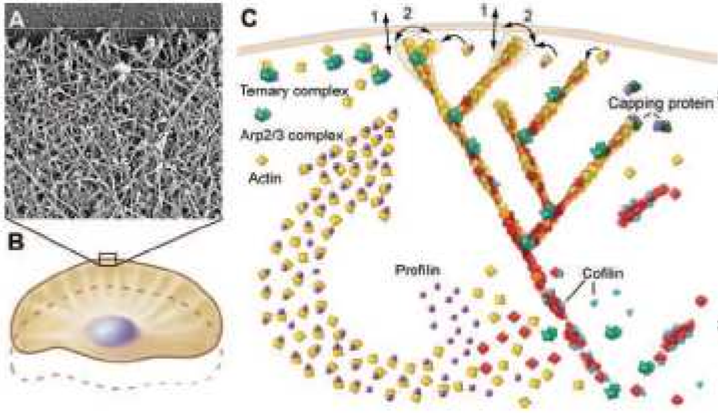
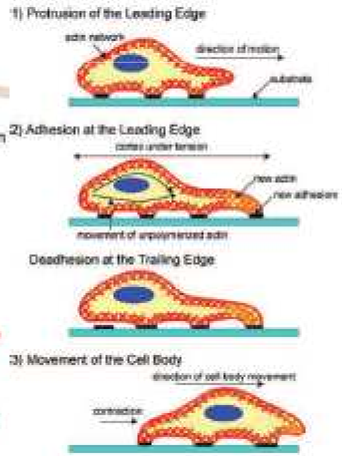


K. Keren et al. (2008)



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



R. Ananthakrishnan and A. Ehrlicher (2003)

keratocyte2.flv

Listeria monocytogenes.mp4

Summer School late September 2011

ISTITUTO NAZIONALE DI ALTA MATEMATICA (INdAM)

GRUPPO NAZIONALE PER LA FISICA MATEMATICA (GNFM)

XXXVI SUMMER SCHOOL ON MATHEMATICAL PHYSICS
(RAVELLO - SEPTEMBER 19 - OCTOBER 1, 2011)

The aim of the school is to give introductive lectures by international experts in the field of Mathematical Physics and Applied Mathematics. The school is mainly addressed to young researchers.
Four courses will be given in a series of 12 lectures scheduled in the morning of each day.

Courses:

1. **Self-gravitating systems, with different aspects and applications** (adhesion dynamics, Vlasov dynamics, statistical equilibria and illustrations in cosmolology, numerics and cold atoms experiments) (6 lectures - I week , Prof. *Y. Brenier - Nice*; 6 lectures - II week, Prof. *J. Barré - Nice*);

2. **Cell motility and self-propulsion in viscous fluids: mechanics and control theoretic approach** (6 lectures - I week, Prof. *A. De Simone - Trieste*; 6 lectures - II week, Prof. *M. Tucsnak - Nancy*);

request by e-mail to gnfm@altamatematica.it not later June 30, 2011.