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

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Drawing from collaborations with:

S. Conti, Bonn; G. Dolzmann, Regensburg; K. Urayama, Kyoto;

A. Di Carlo and L. Teresi, Roma Tre; **V. Agostiniani**, **P. Cesana**, Trieste.

Workshop on Macroscopic Modeling of Materials with Fine Structure, CMU, May 27, 2011

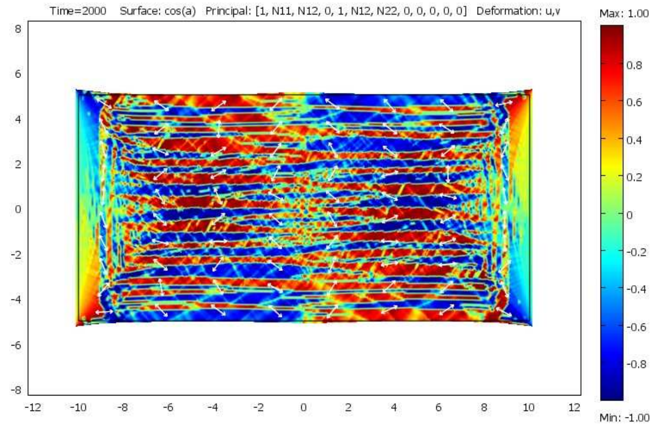
Outline

[Part 1](#)

Introduction to nematic elastomers: the key experiments.

Part 2

Energy-based models for nematic elastomers.



Part 3

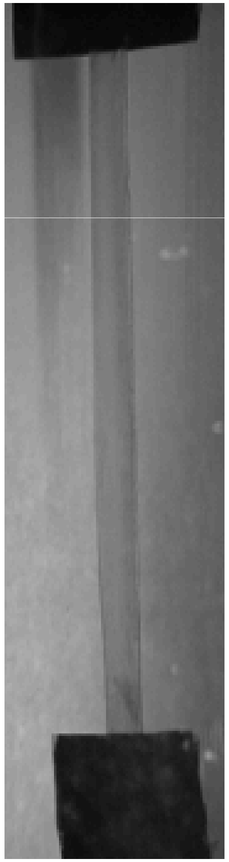
Numerical simulation of the key experiments.

Part 4

Small strain theory, dynamics under an applied electric field

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



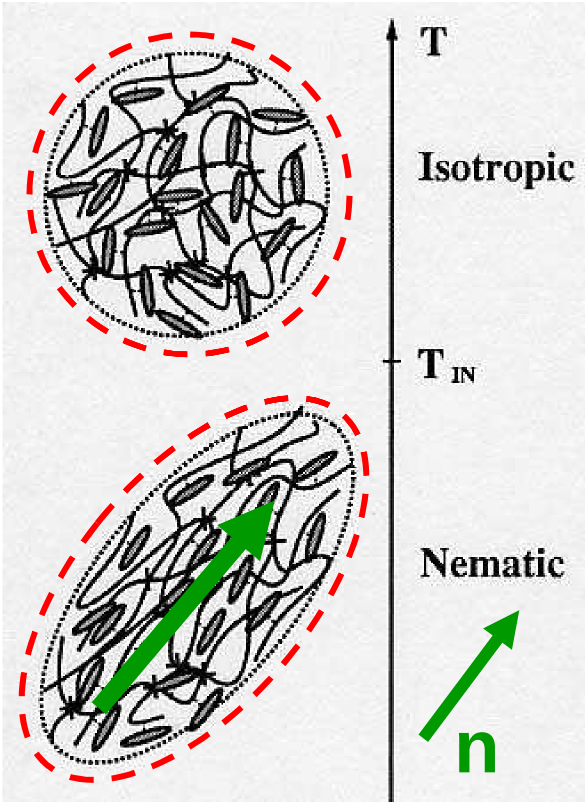
(H. Finkelmann)

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 $a^{1/3} \geq 1$ $(a > 1)$

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

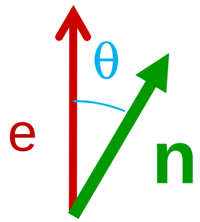


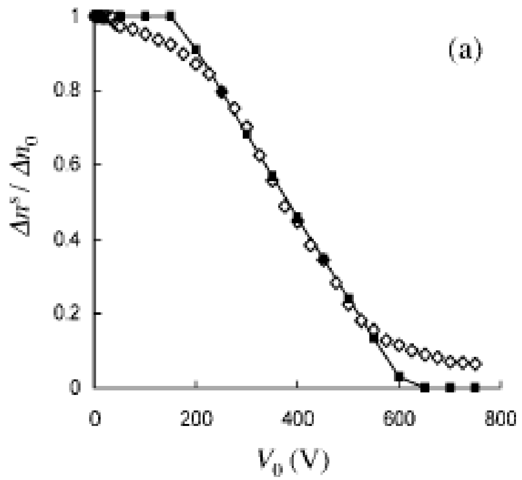
Electro-mech coupling: align with e field.

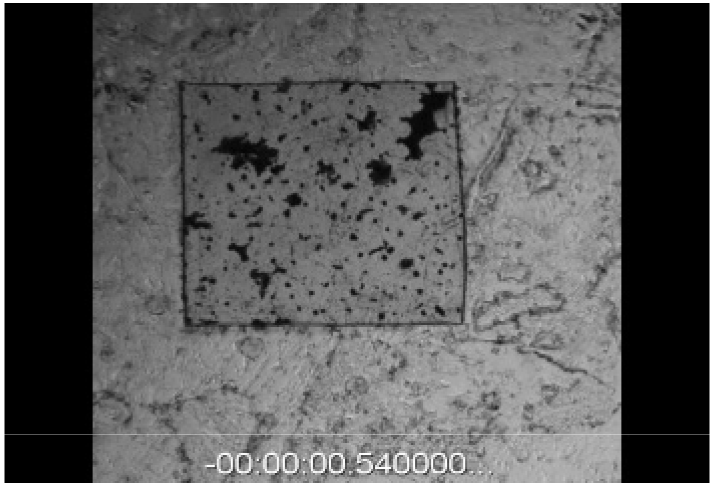
(from now on: fixed temperature in nematic phase)

equil. opitcal birefringence

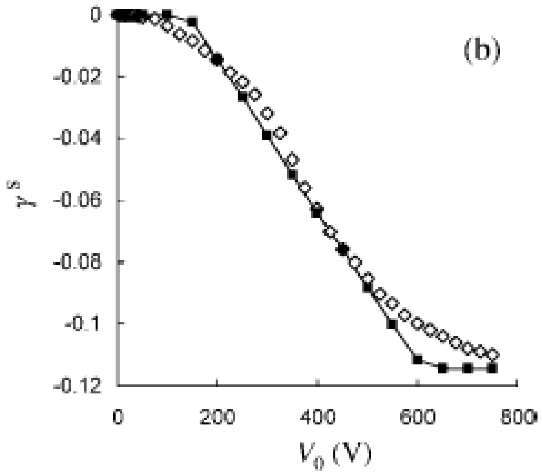
$\cos^2(\theta)$

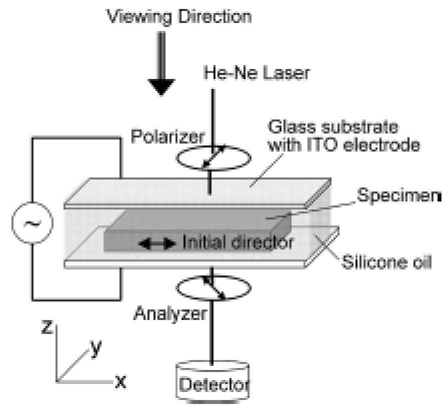






equil. horizontal strain



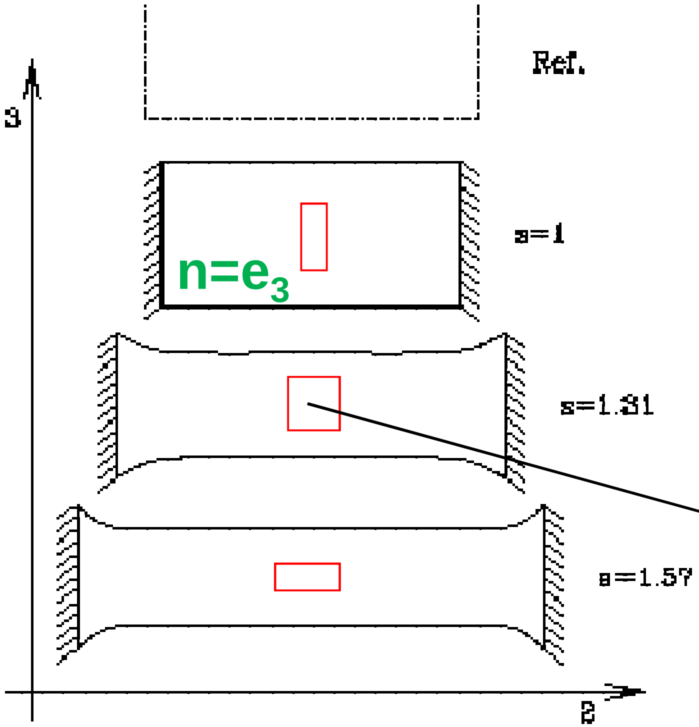


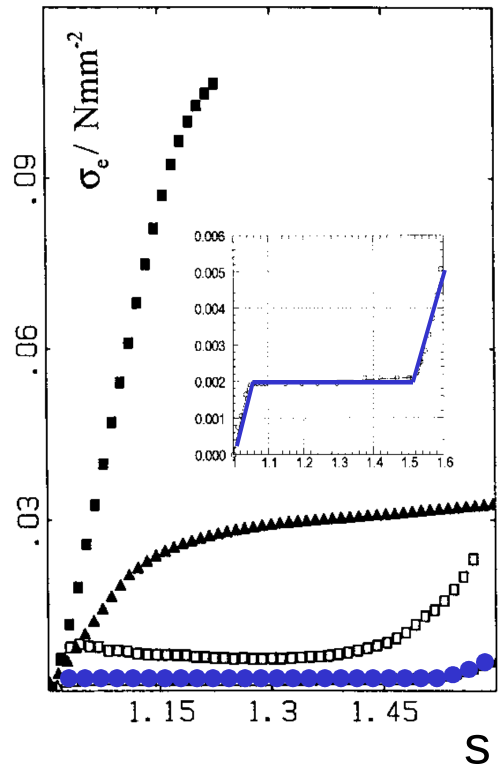
A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi:
Dynamics of electro-opto-mechanical effects in swollen nematic elastomers, Macromolecules, vol.41, p. 9389 (2008).

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)





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

(H. Finkelmann, 95)

Summary from Part 1

- Isotropic-To-Nematic phase transformation:
  the spontaneous strain $F_n = a^{1/3}\, n\otimes n + a^{-1/6}(I - n\otimes n)$

- Dielectric anisotropy:
  n aligns with e-field, strain accompanies director rotation

- Purely mechanical stetching:
  existence of a plateau in stress-strain response
  director rotation accompanies plateau
  director rotation in clamped geometry may be nonuniform

Part 2: energy based model

The lesson from martensites: relevance of spontaneous strains

- Cristallographic theory of martensites.
  Geometry of patterns dictated by kinematic compatibility between variants.

- Energy-based view:
  tend to see only martensitic variants because they are low energy states.

The model for nematic elastomers:

- What are the low energy states?
  (zeros of energy density = Bain strain and material symmetry)

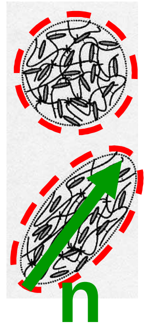
- How does the energy grow away from them?
  (functional form of the energy density)

A. DeSimone: Energetics of fine domain structures in nematic elastomers, Ferroelectrics, vol. 222, p. 275 (1999).

Warner-Terentjev energy, and corrections

M. Warner, E. Terentjev, Liquid crystal elastomers, Clarendon Press, Oxford 2003.

$W(F, n) = \frac{1}{2}\mu\,(F F^T) \bullet (F_n F_n^T)^{-1}$, det F=1



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

W is minimized iff $F F^T = F_n F_n^T$ i.e.

singular values of F must be $a^{1/3}$, $a^{-1/6}$, $a^{-1/6}$. and n = max stretch direction.

This density is isotropic (no memory of cross-linking state):

- $\min_n W(F,n) = \frac{1}{2}\mu\,(\lambda_{min}^2 + \lambda_{int}^2 + \lambda_{max}^2 / a)$ λ principal stretches

  (**n** must be aligned with the current direction of maximal stretch)

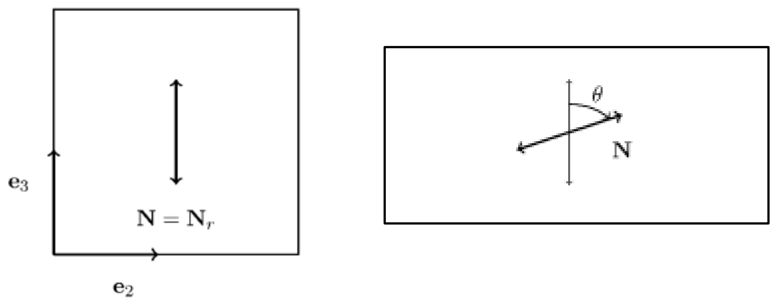
- F_n is an isotropic function of n: $F_{Rn} = R F_n R^T$

Anisotropic corrections: W_α, W_β, ... (favoring special director n_o)

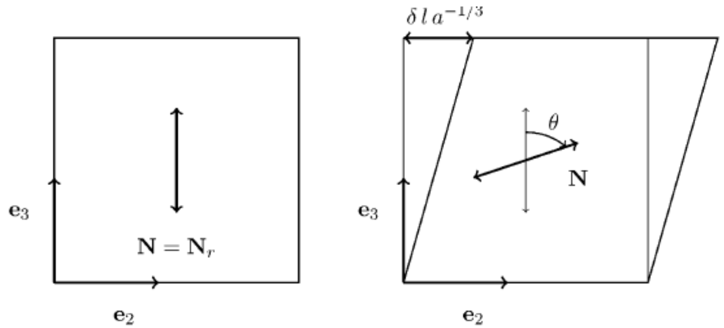
Also: Frank elasticity, electrostatic energy, ...

Explore energy landscape through homogeneous stretch and shear: instabilities

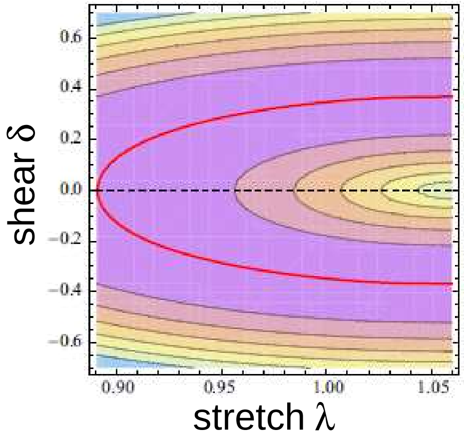
Stretch by λ

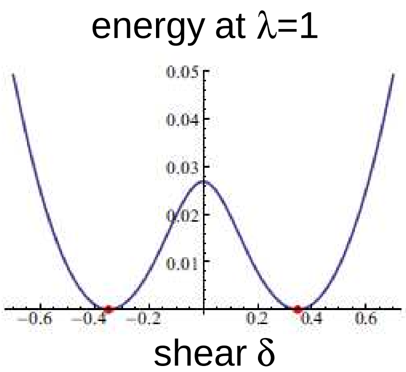


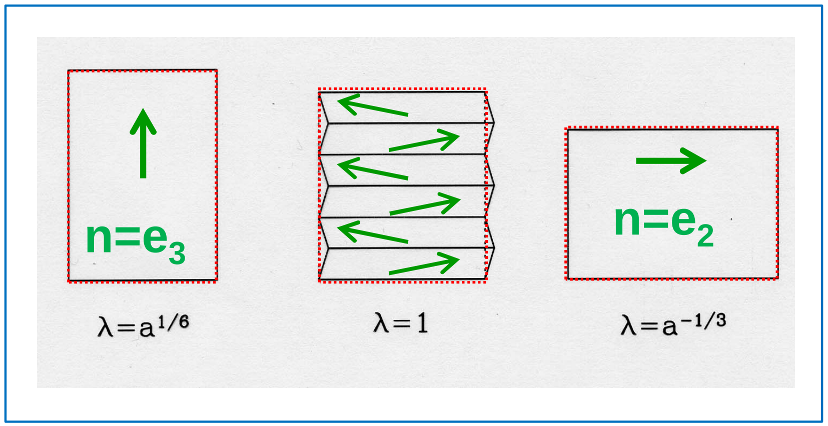
Shear by δ



$\underset{n}{\text{Min}}$ W (F,n) (isotropic)

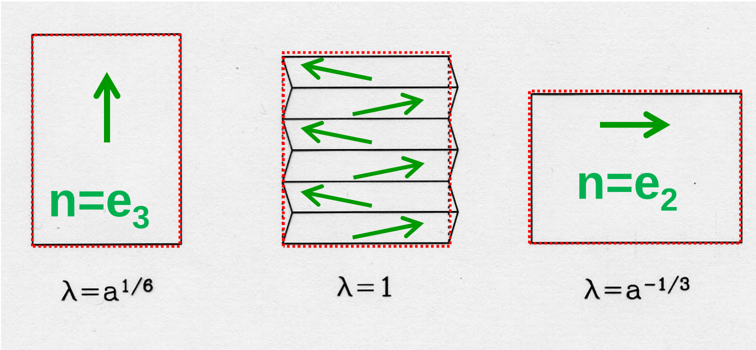




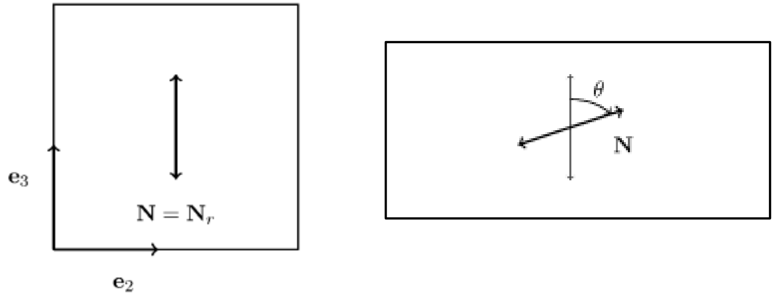


M. Warner, E. Terentjev, Liquid crystal elastomers, Clarendon Press, Oxford 2003.
A. DeSimone, L. Teresi: Elastic energies for nematic elastomers, Eur. Phys. J. E, vol. 29, p. 191 (2009).

Similar instabilities for anisotropic energy

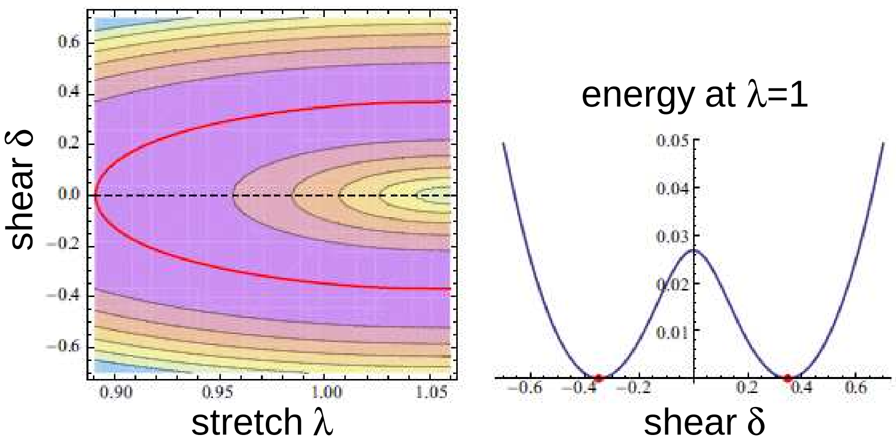


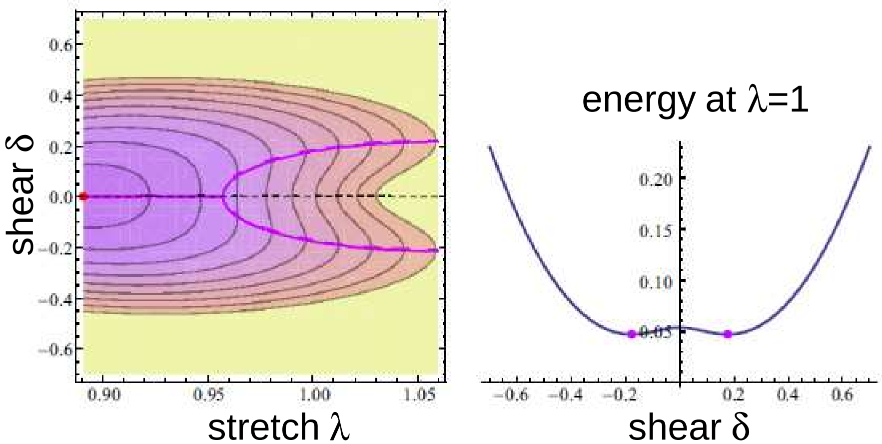
Stretch by λ



$\min_{n} W(F,n)$ (isotropic)

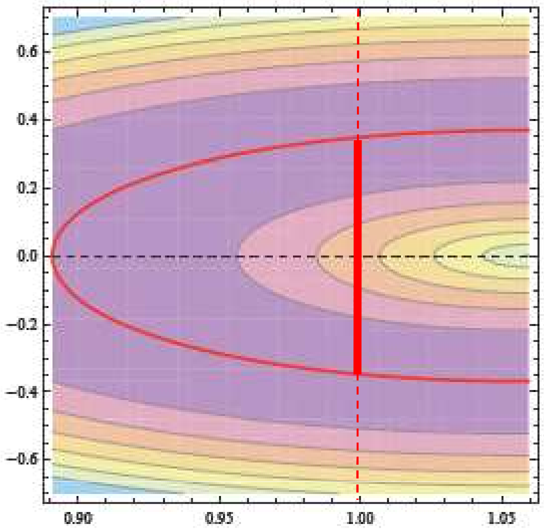
$\min_{n} W_\beta(F,n)$ (anisotropic)

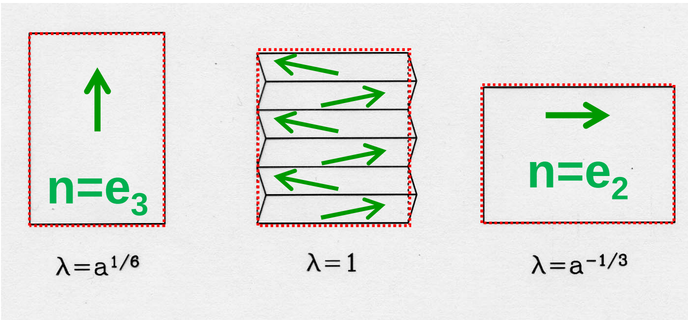


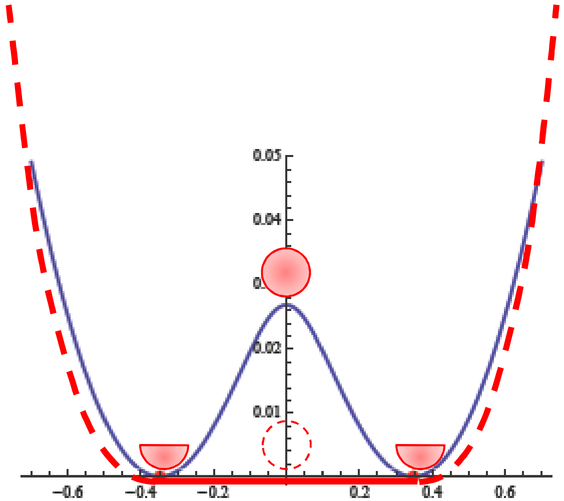


A. DeSimone, L. Teresi: Elastic energies for nematic elastomers, Eur. Phys. J. E, vol. 29, p. 191 (2009).

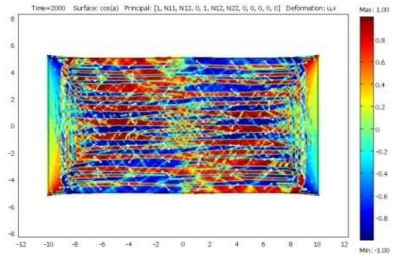
A coarse-grained model based on minimizing effective energy





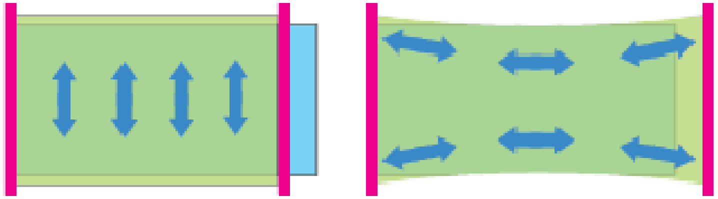


Effective macroscopic energy (quasi-convex envelope)



Can turn this into a computational strategy: avoid resolving fine scales explicitly, though they are accounted for in the energetics (homogenization, relaxation ...)

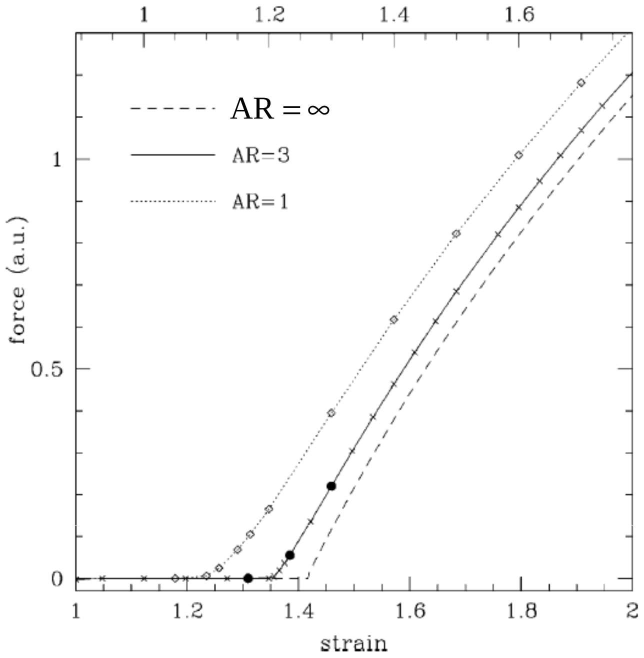
Part 3: Numerical stretching experiments

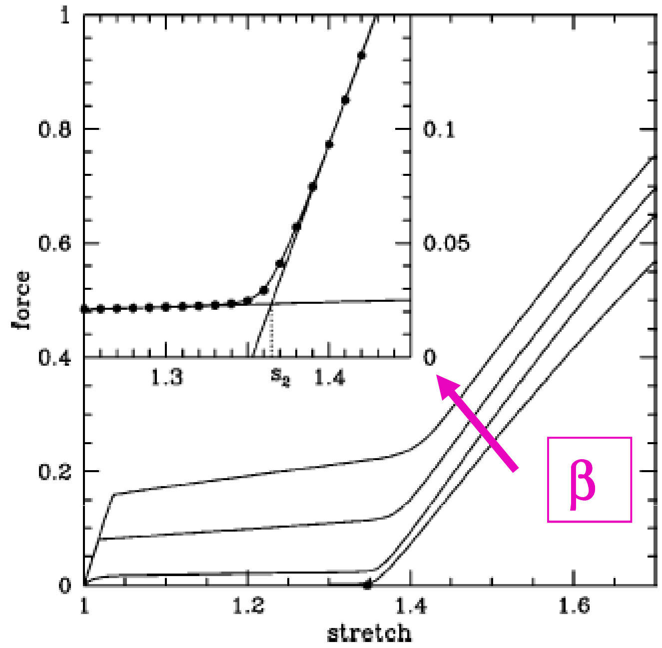


Type 1: For each prescribed end displacement, compute energy minimizing state (a one-parameter family of minimization problems)

Type 2: Assign time-dependent end displacements and solve for the dynamics (necessary to explore rate-dependence of stress-strain response)

Force-stretch curves from energy minimizing states through qc envelopes



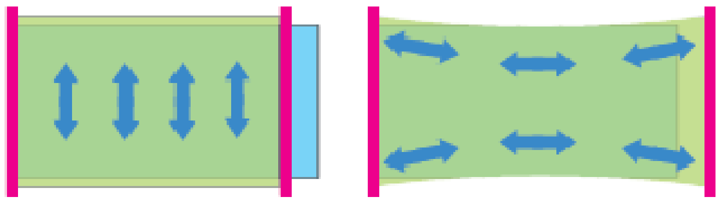


$\min_n W(F,n)$

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

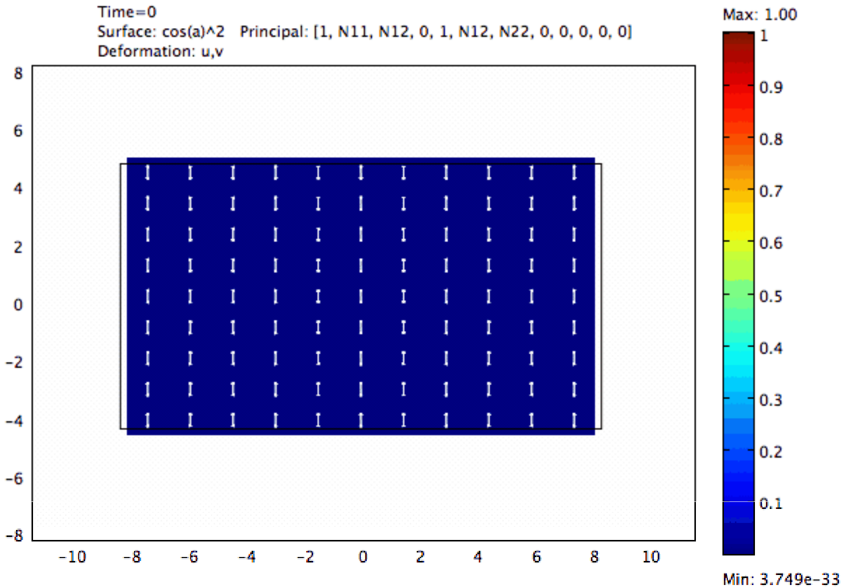
isotropic: no memory of n at cross-linking

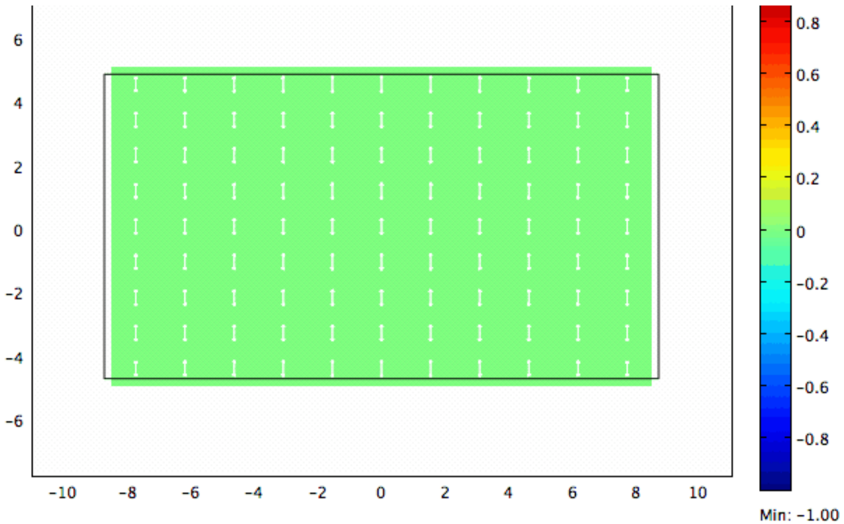
β strength of anisotropy

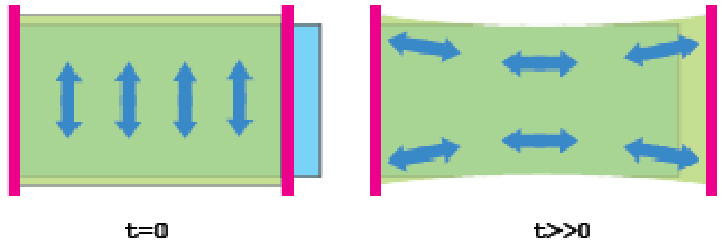


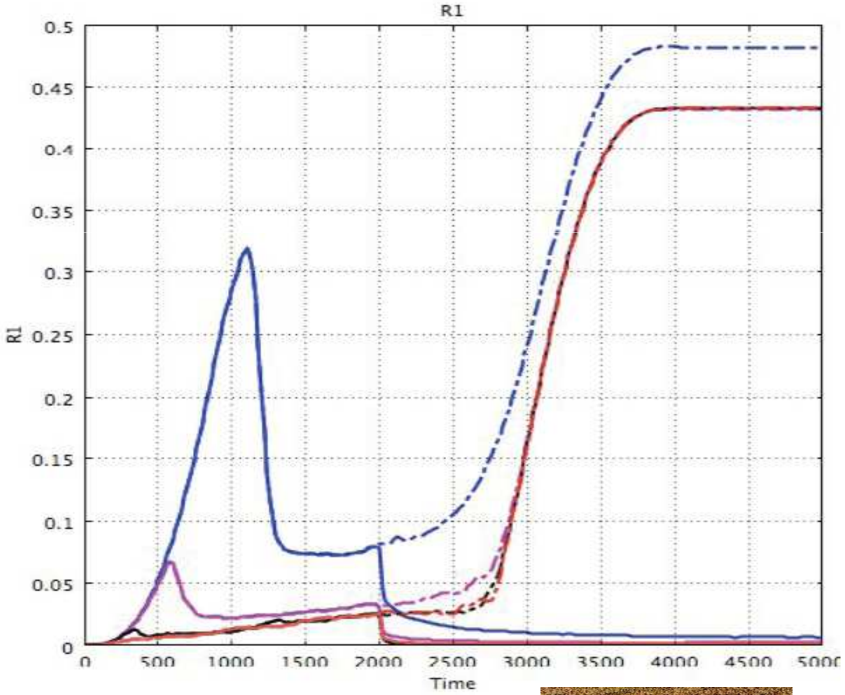
S. Conti, A. DeSimone, G. Dolzmann:
Soft elastic response of stretched sheets of nematic elastomers: a numerical study, J. Mech. Phys. Solids, vol.50, p. 1431 (2002);
Semi-soft elasticity and director reorientation in stretched sheets of nematic elastomers, Phys. Rev. E, vol. 66, p. 061710 (2002).

Dynamics and dependence of force-stretch curves on stretching rate







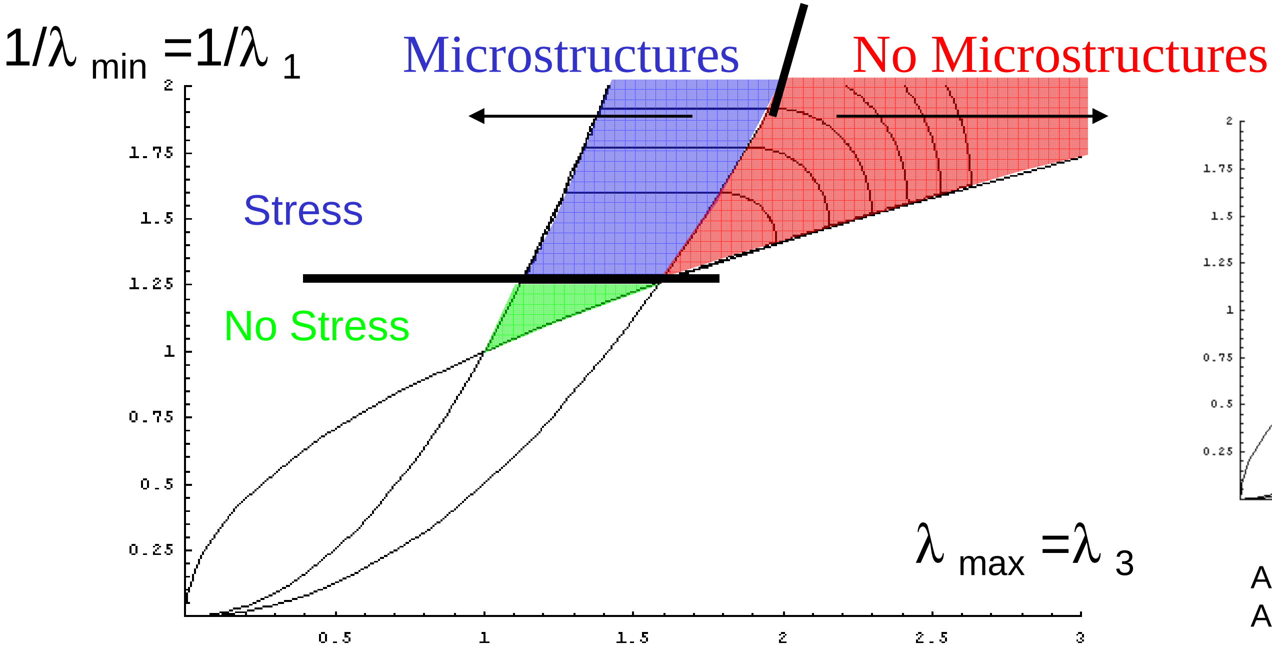


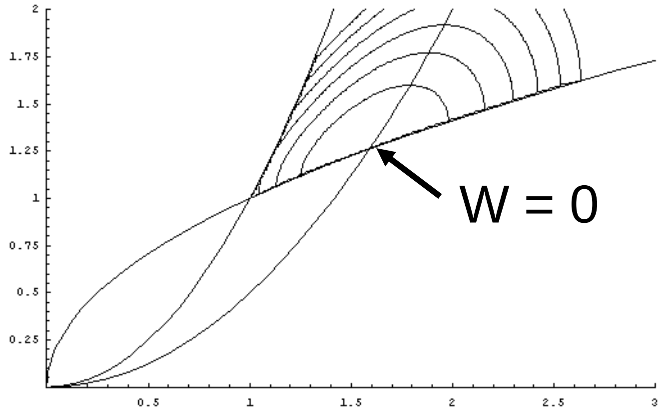
Some details.....

The quasi-convexified energy W^{qc}

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

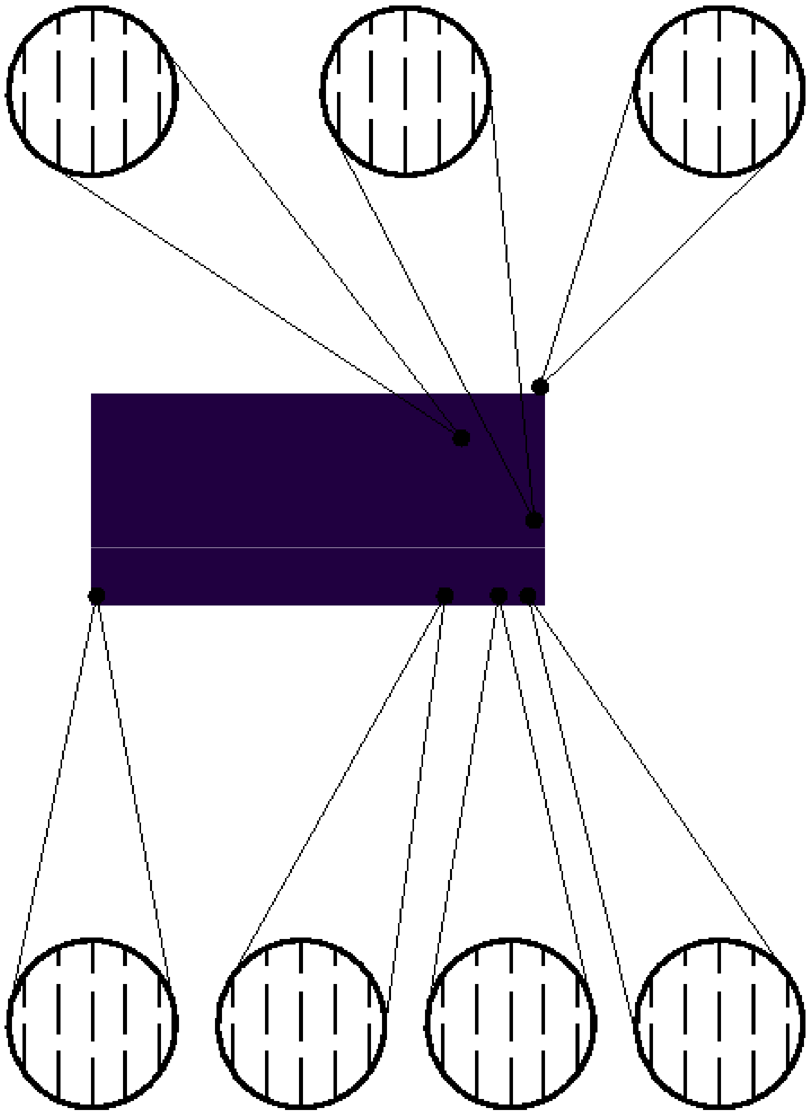
if $\det F = 1$, $W^{qc}(F) = +\infty$ if $\det F \neq 1$.

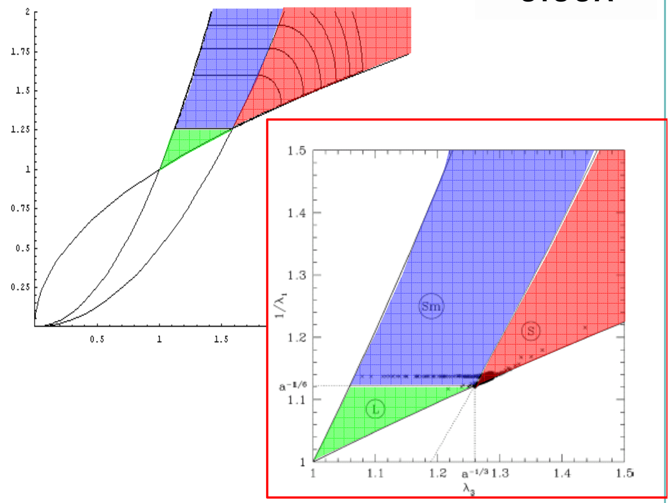


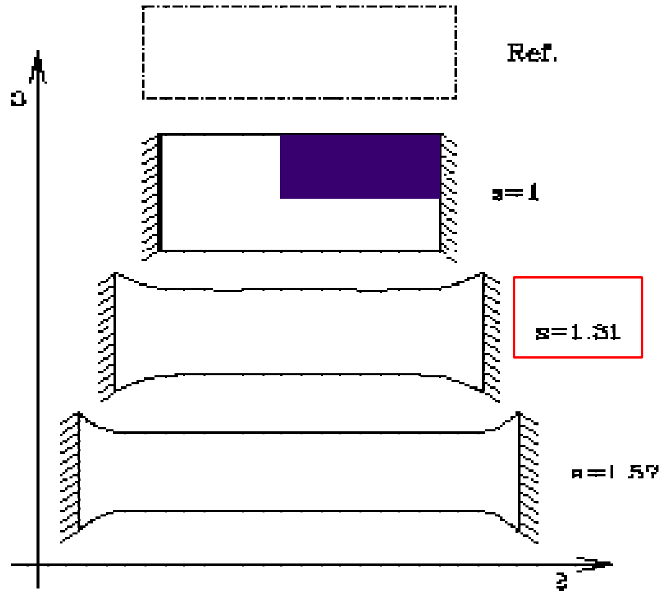


A. DeSimone, G. Dolzmann:
Arch. Rat. Mech. An., vol.161, p.181 (2002).

Use W^{qc} in numerical stretching experiment





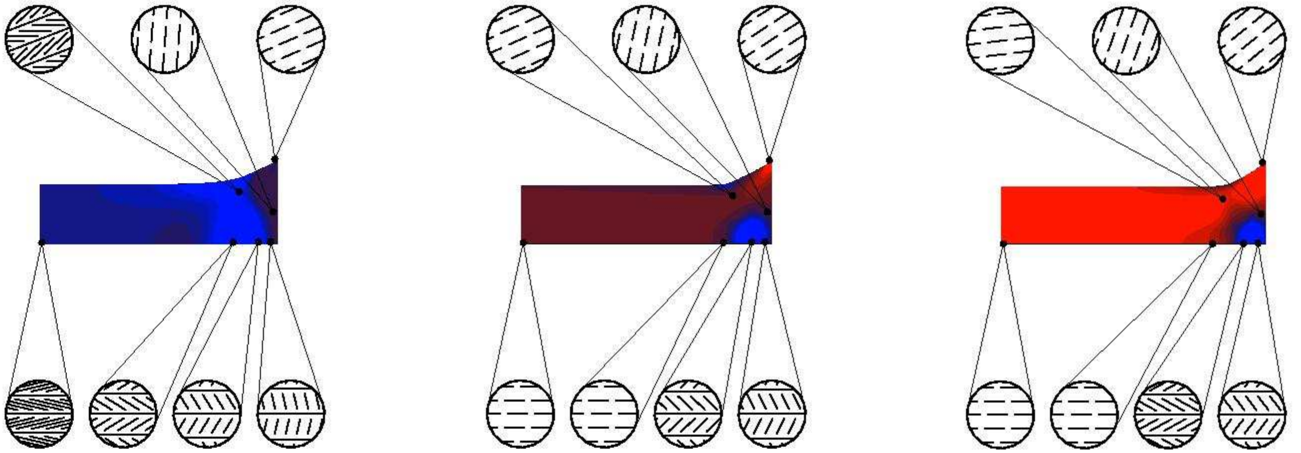


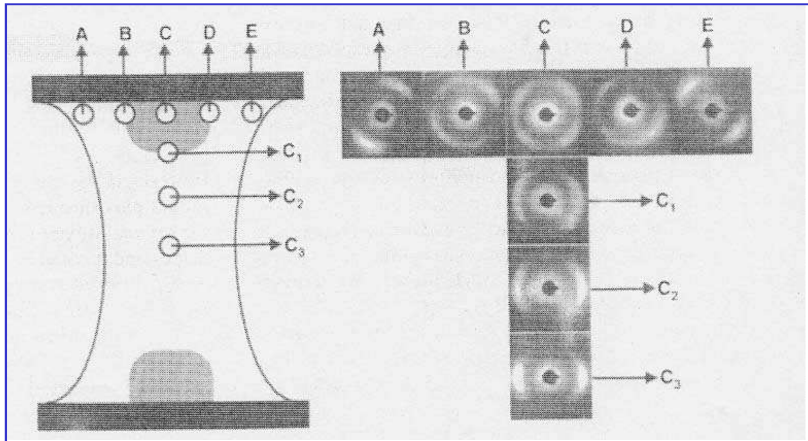
S. Conti, A. DeSimone, G. Dolzmann:
J. Mech. Phys. Solids, vol.50, p. 1431 (2002).

Theory vs. Experiment

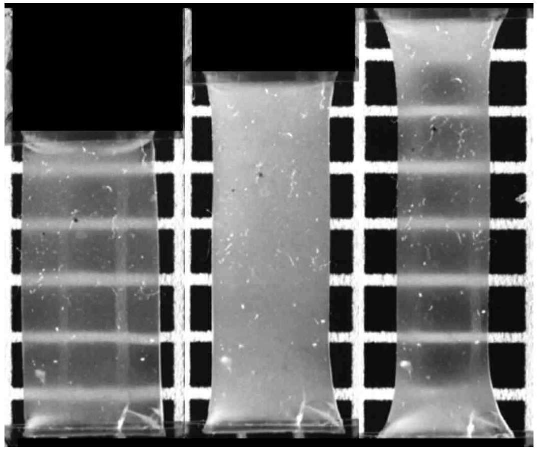
Multiscale numerics

(Conti, DeSimone, Dolzmann)





X-ray scattering (Zubarev et al.)



Direct observation (Terentjev)

Part 4: Small strain theory

Can use small strain theory as well

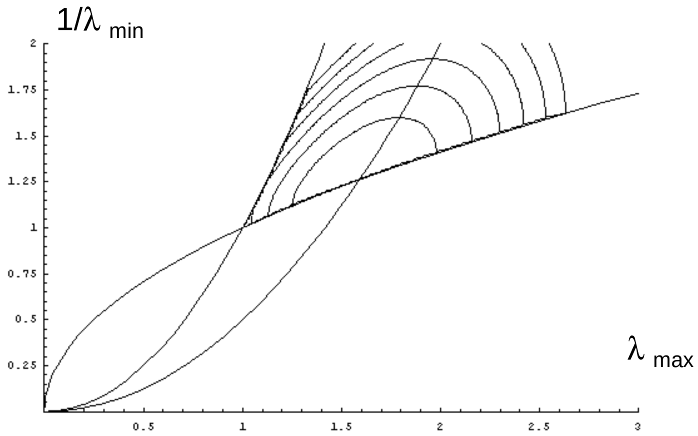
$a^{1/3} = 1 + \gamma\,,\ \ \gamma \ll 1$

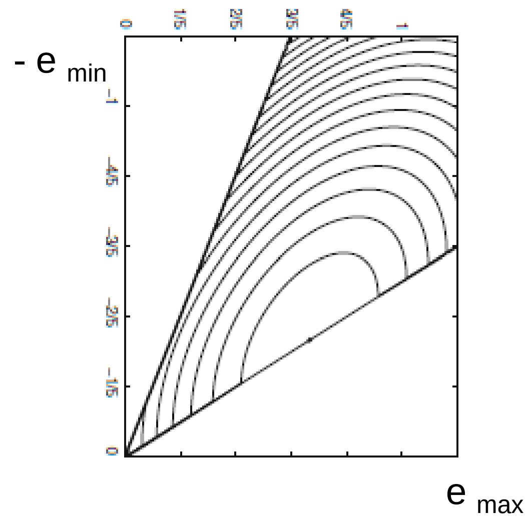
measures spontaneous stretch along n

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

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

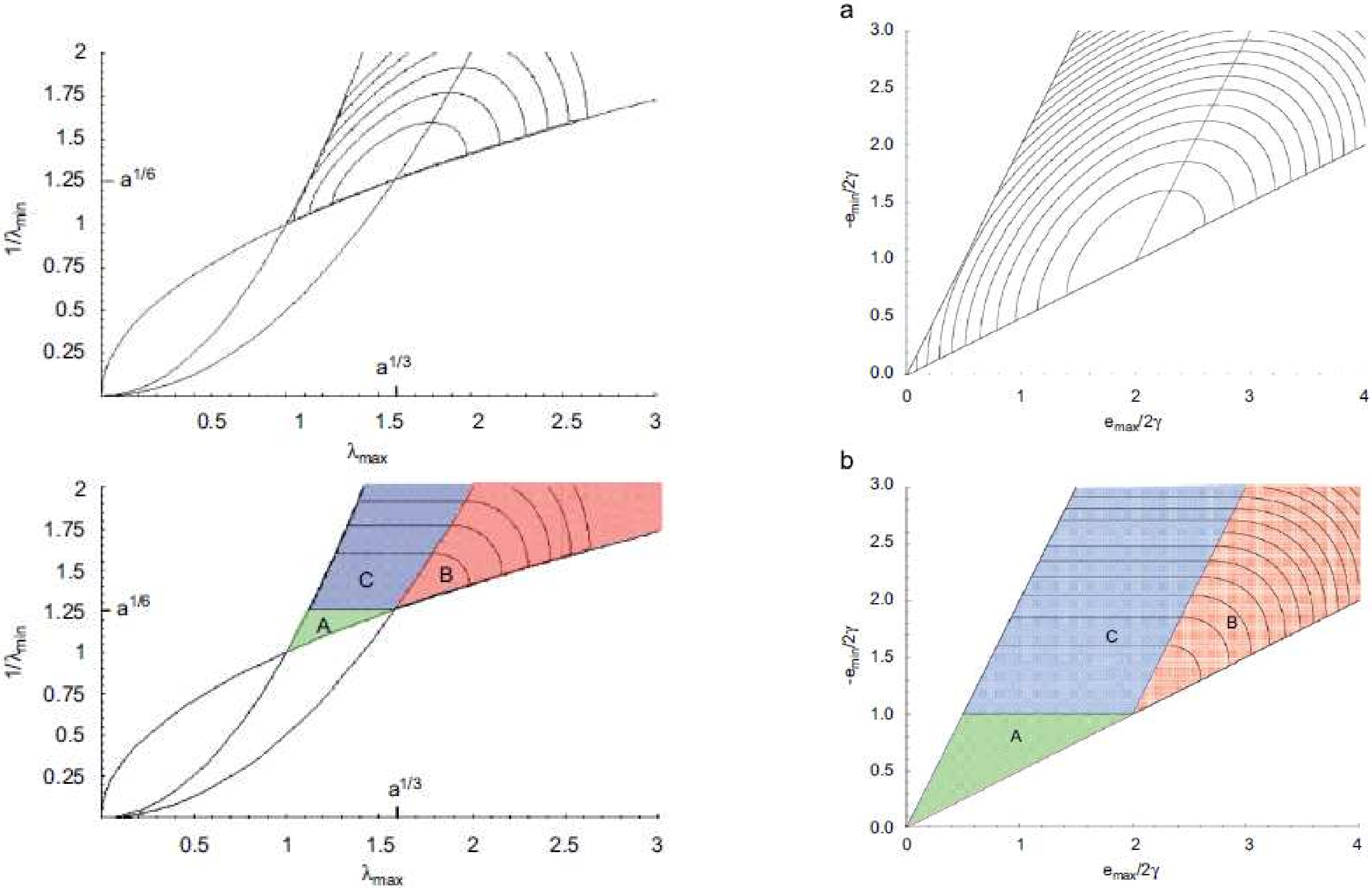
$$W(F,n) = ½\,\mu\,(F\,F^T)\bullet(F_n\,F_n^T)^{-1} \longrightarrow \mu\,|\,E - E_0(n)\,|^2$$





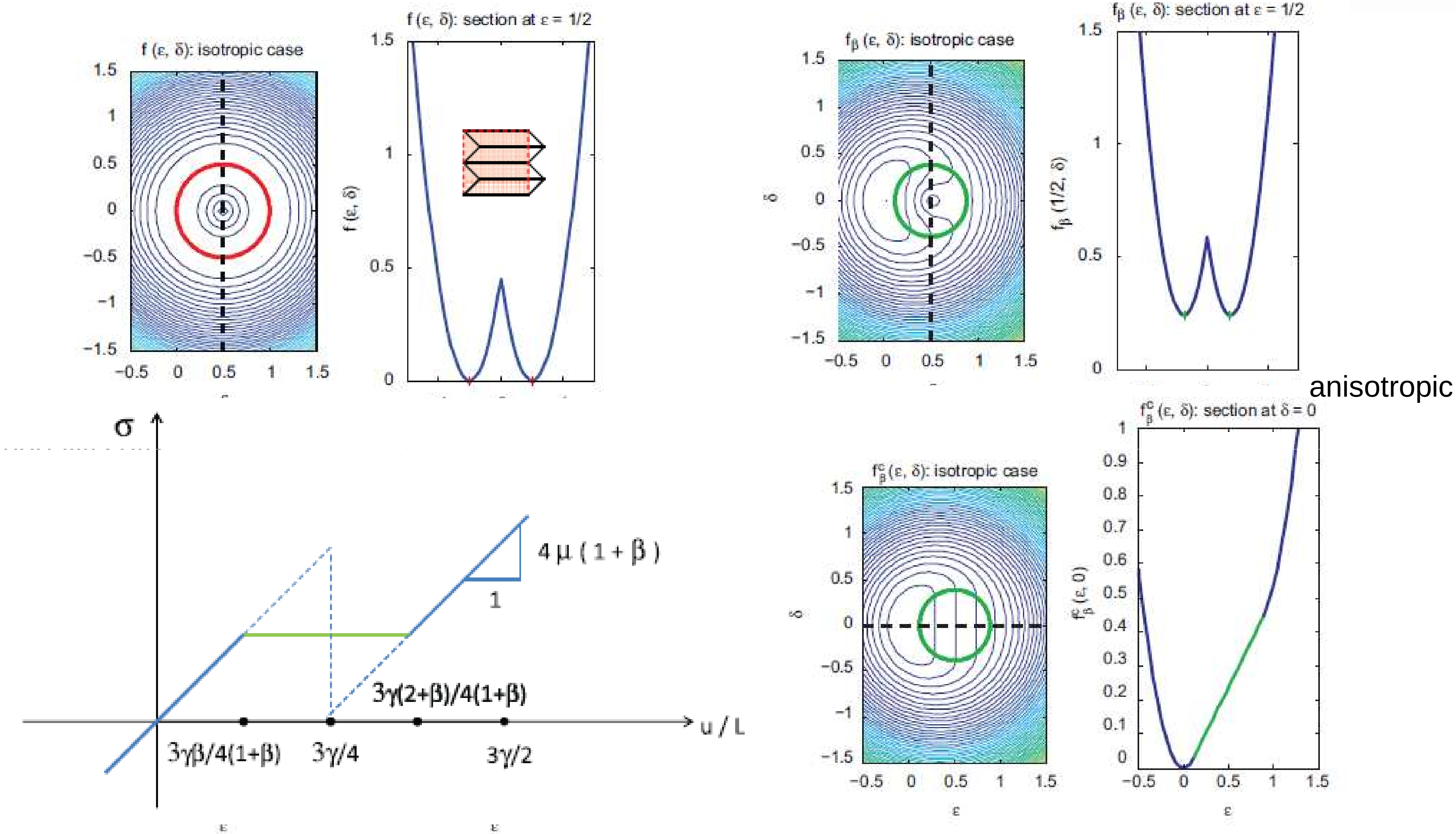
A. DeSimone, L. Teresi: Elastic energies for nematic elastomers, Eur. Phys. J. E, vol. 29, p. 191 (2009). P. Cesana: Relaxation of multiwell energies, Arch. Rat. Mech. Anal. (2010). V. Agostiniani, A. DeSimone: Gamma-convergence of energies for nematic elastomers in the small strain limit, Cont. Mech. Thermodyn. Vol. 23, p. 257 (2011).

QC envelopes (3d)



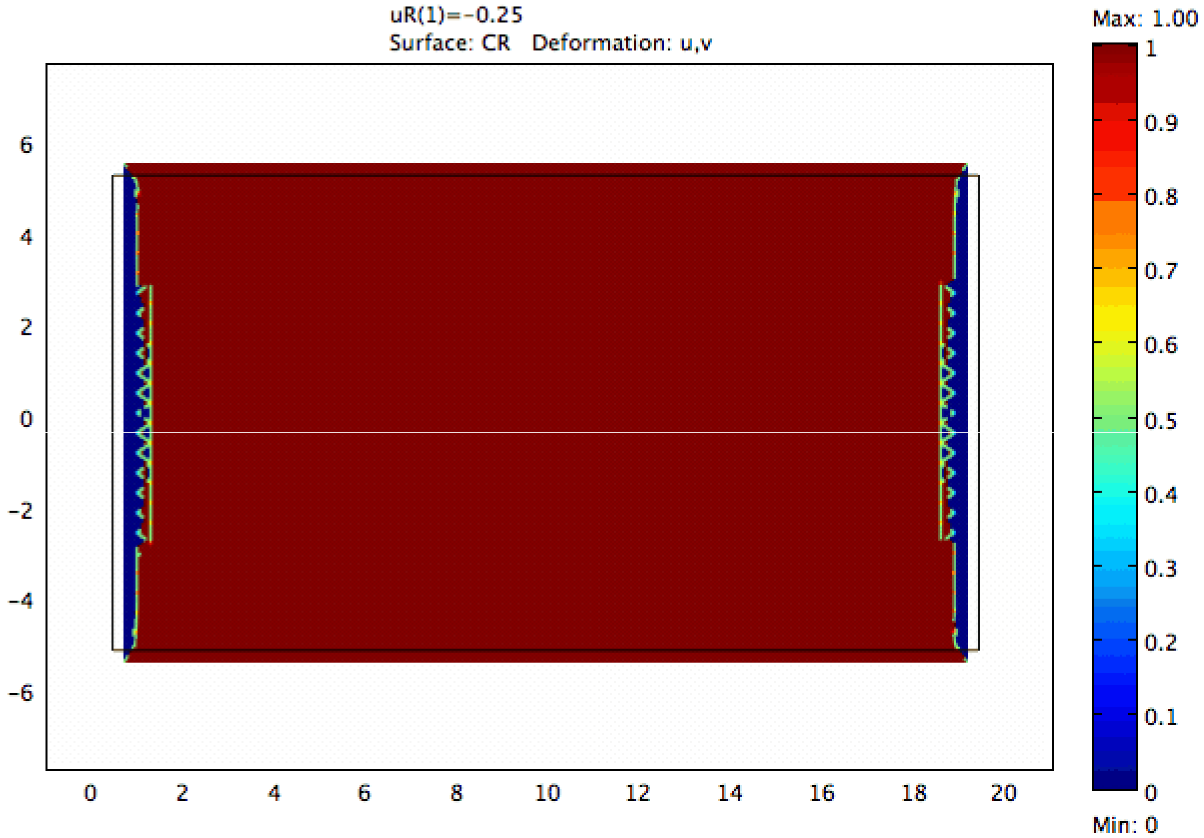
P. Cesana, Relaxation of multiwell energies in linearized elasticity and application to nematic elastomers, Archive Rat. Mech. Analysis (2010); P. Cesana and A. DeSimone, Quasiconvex envelopes of energies for nematic elastomers in the small strain regime and applications, J. Mech. Phys. Solids, vol. 59, p. 787 (2011).

QC envelopes (plane strain, extension-shear)



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).

Numerics with small strain theory



Dynamics under Electric Field

$$\mathcal{E} = \frac{1}{2}\int_{\mathcal{B}} \left(k_F |\nabla \mathbf{n}|^2 + \mathbb{C}\,(\mathbf{E}_{\mathbf{u}} - \mathbf{E}_0)\cdot(\mathbf{E}_{\mathbf{u}} - \mathbf{E}_0)\right)$$

$$-\frac{1}{2}\int_{\Omega} \left(\varepsilon_o (\mathbb{D}\,\nabla\varphi)\cdot\nabla\varphi \right) - \int_{\partial_s \mathcal{B}} (\mathbf{s}_{ext}\cdot\mathbf{u})\,,$$

$E_0=E_0(n)$, $C=C(n)$, $D=D(n)=\varepsilon_0\,(\varepsilon_a\, n\otimes n + \varepsilon_\perp I)$

$$0 = \frac{\delta\mathcal{E}}{\delta\varphi}$$

$$\frac{\delta\mathcal{D}}{\delta\dot{\mathbf{u}}} = -\frac{\delta\mathcal{E}}{\delta\mathbf{u}}$$

$$\frac{\delta\mathcal{D}}{\delta\dot{\mathbf{n}}} = -\frac{\delta\mathcal{E}}{\delta\mathbf{n}}$$

$$\mathrm{div}\,(\mathbf{d}) = 0 \qquad \mathbf{d} = -\varepsilon_o\,\mathbb{D}\nabla\varphi$$

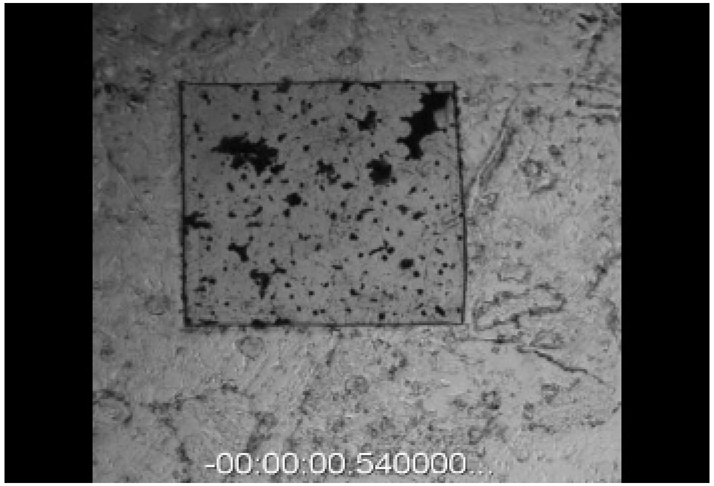
$$\mathrm{div}\,(\mathbb{S}) = 0 \qquad \mathbb{S} = \mathbb{C}\,(\mathbb{E}_{\mathbf{u}} - \mathbb{E}_0) + \eta_g \mathbb{E}_{\dot{\mathbf{u}}}$$

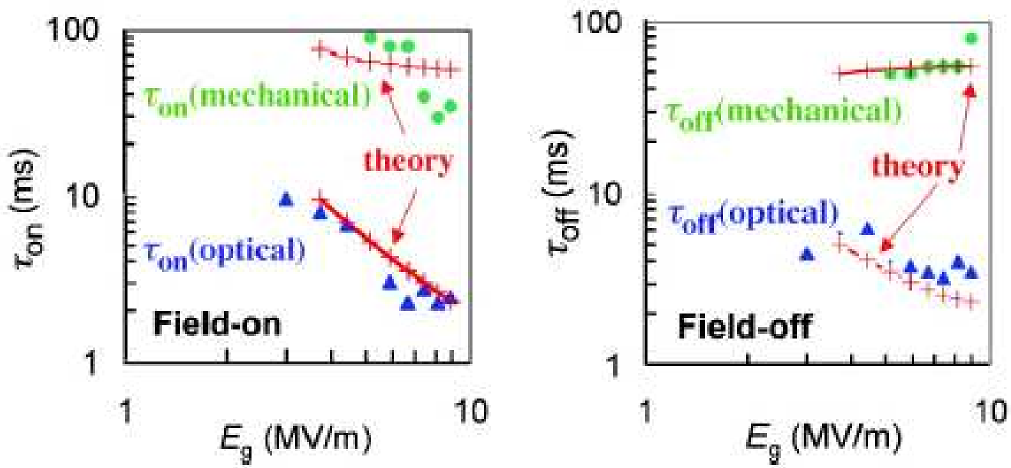
$$\eta_n(\dot{\mathbb{R}}\mathbb{R}^T - \mathbb{W}_{\dot{\mathbf{u}}}) = [\mathbb{S}_e\,,\mathbb{E}_0] + \frac{1}{2}\varepsilon_o\varepsilon_a[\nabla\varphi\otimes\nabla\varphi\,,\mathbf{n}\otimes\mathbf{n}] + \mathrm{skw}\,(\mathrm{div}\,(k_F\nabla\mathbf{n})\otimes\mathbf{n})$$

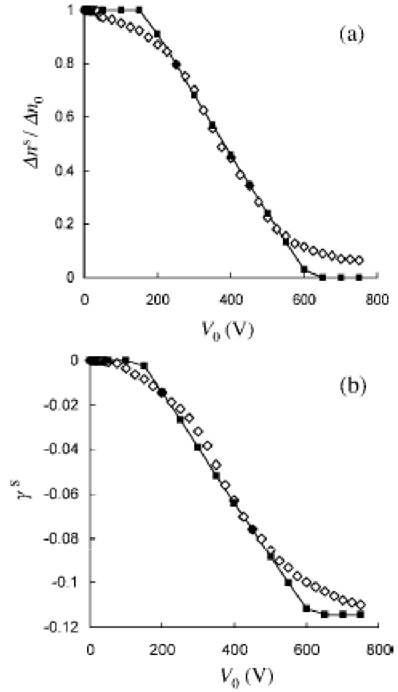
As for purely mechanical stretching, need to add anisotropy to get realistic results !

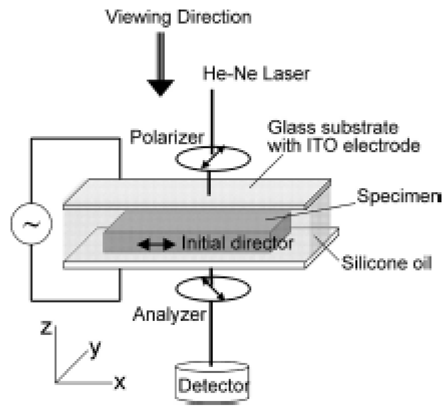
A. DeSimone, A. DiCarlo, L. Teresi: Critical voltages and blocking stresses in nematic gels, Eur. Phys. J. E, vol. 24, p. 303 (2007).

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





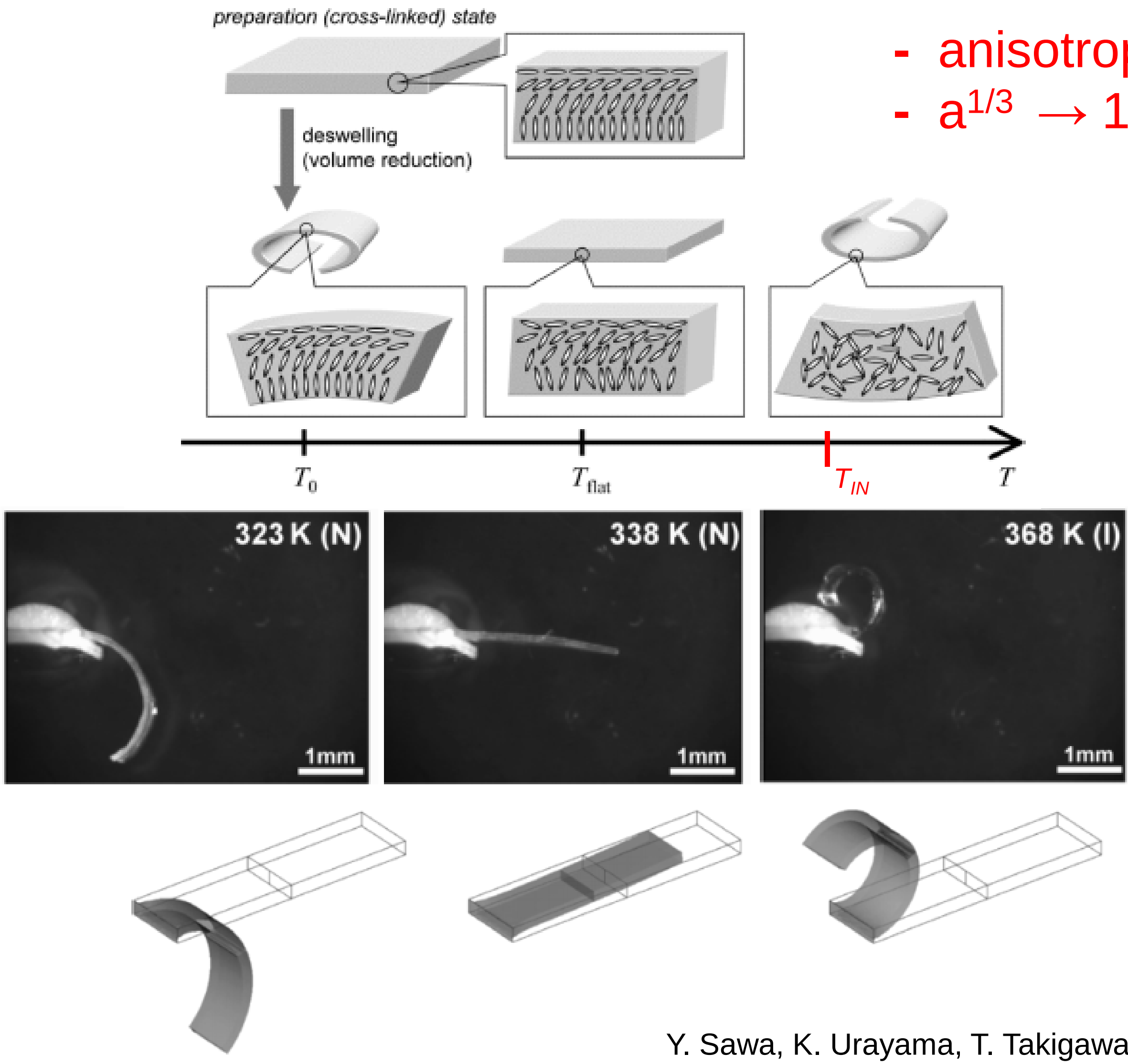




A. Fukunaga, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi:
Dynamics of electro-opto-mechanical effects in swollen nematic elastomers, Macromolecules, vol.41, p. 9389 (2008).

Patterned nematic texture (soft manipulator)

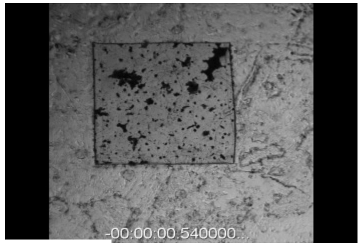
- anisotropic swelling
- $a^{1/3} \rightarrow 1$ as $T \rightarrow T_{IN}$



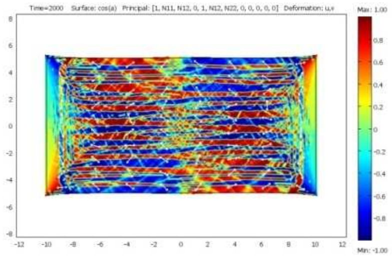
Y. Sawa, K. Urayama, T. Takigawa, A. DeSimone, L. Teresi: Thermally driven giant bending of LCE films with hybrid alignment, Macromolecules, vol.43, p. 4362 (2010).

Conclusions

An interesting model system. Applications?
(soft contractile actuators: microfluidics, artificial muscles?)

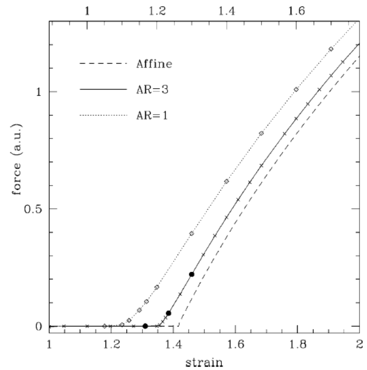


A very rich system to explore material response from evolving microstructures

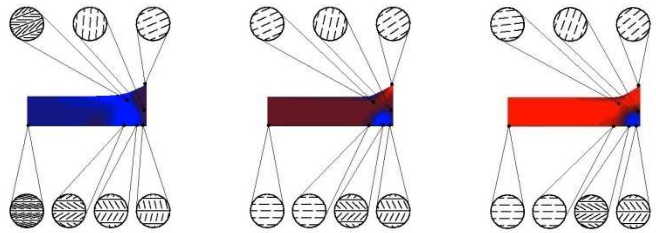


In particular:

Dependence of “constitutive” response on sample size, aspect ratio, details of loading device,...



Coarse grained models based on convexified energies useful to predict stress-strain behavior and features of the electromechanical response
(useful also for other materials: M-SMA ... ?)



Dynamic attainability of low energy states ?
Use of patterning to produce useful macro defs.?

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Many contributions by many other authors.....

Monograph:

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