European Laboratory for
Non-Linear Spectroscopy

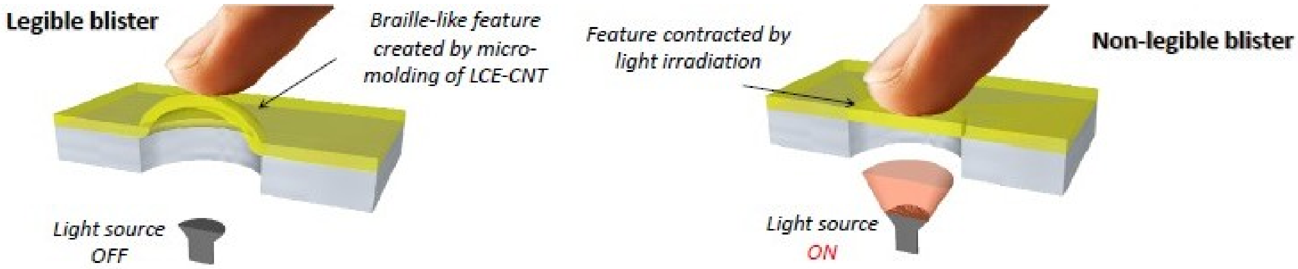
Modelling of the photo-mechanical response of liquid-crystal elastomers

Giacomo Cerretti

Comsol Conference 10-12 October 2012 Milan

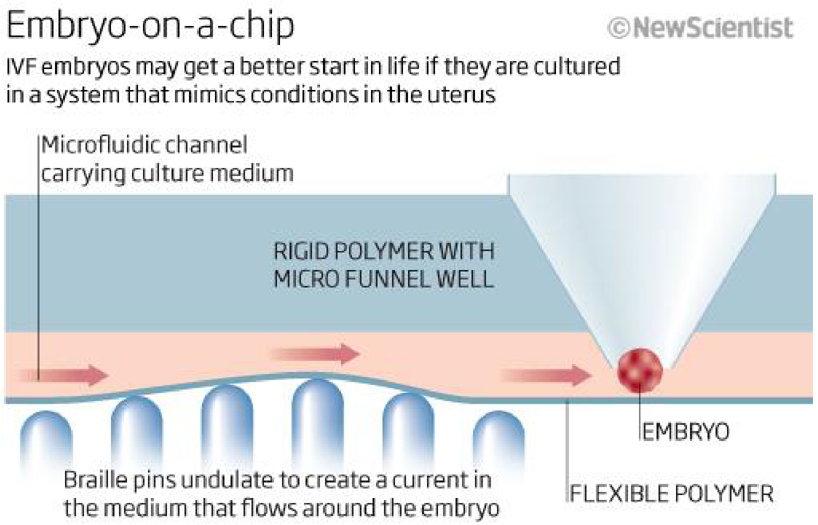
Excerpt from the Proceedings of the 2012 COMSOL Conference in Milan

APPLICATIONS



Braille touchscreens **(Camargo, et al., 2011)**

Soft motors **(Yamada, et al., 2008)**


Embryo-on-a-chip

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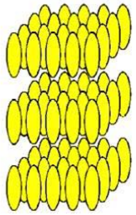
IVF embryos may get a better start in life if they are cultured in a system that mimics conditions in the uterus

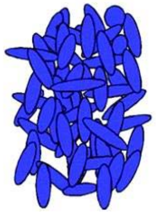
Braille pins undulate to create a current in the medium that flows around the embryo

Embrio-on-a-chip **(Hamzelou, 2011)**

LIQUID CRYSTAL ELASTOMER (LCE)

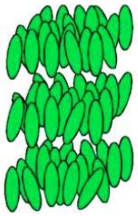


Solid
crystal



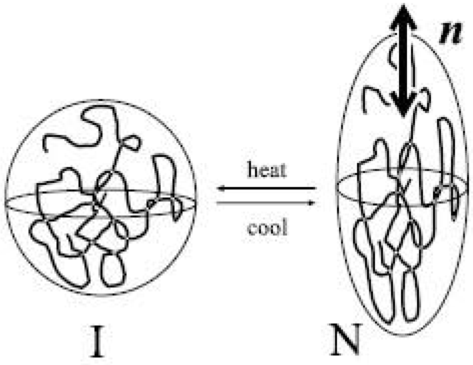
Liquid

(Shakhashiri, 2007)



Liquid
crystal

Nematic phase



(Warner & Terentjev, 2007)

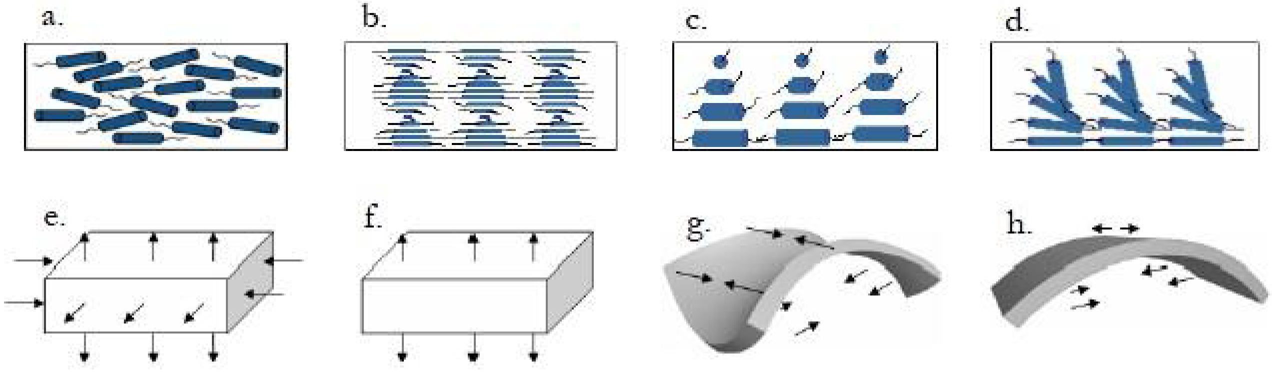
Long polymer chains

Nematically order

LCE

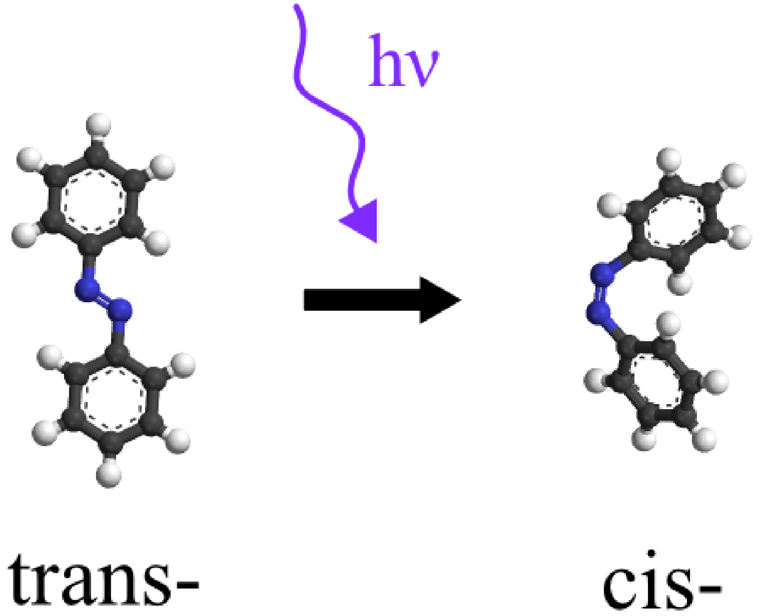
Molecular orderings:

a) Uniaxial
b) Cholesteric
c) Twisted
d) Splayed



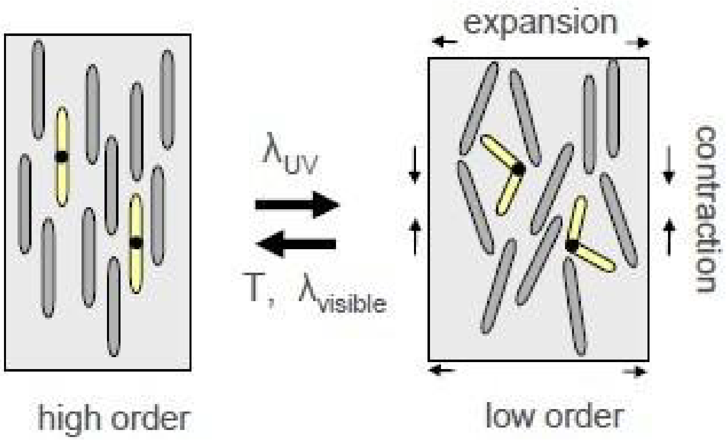
(van Oosten, 2009)

TRANS-CIS ISOMERIZATION



When azobenzene (photoisomerizing dye) absorbs a photon, its molecules change from an elongated trans-state to a bent cis-state.

Photoisomerization of azobenzene causes the light-induced deformation.

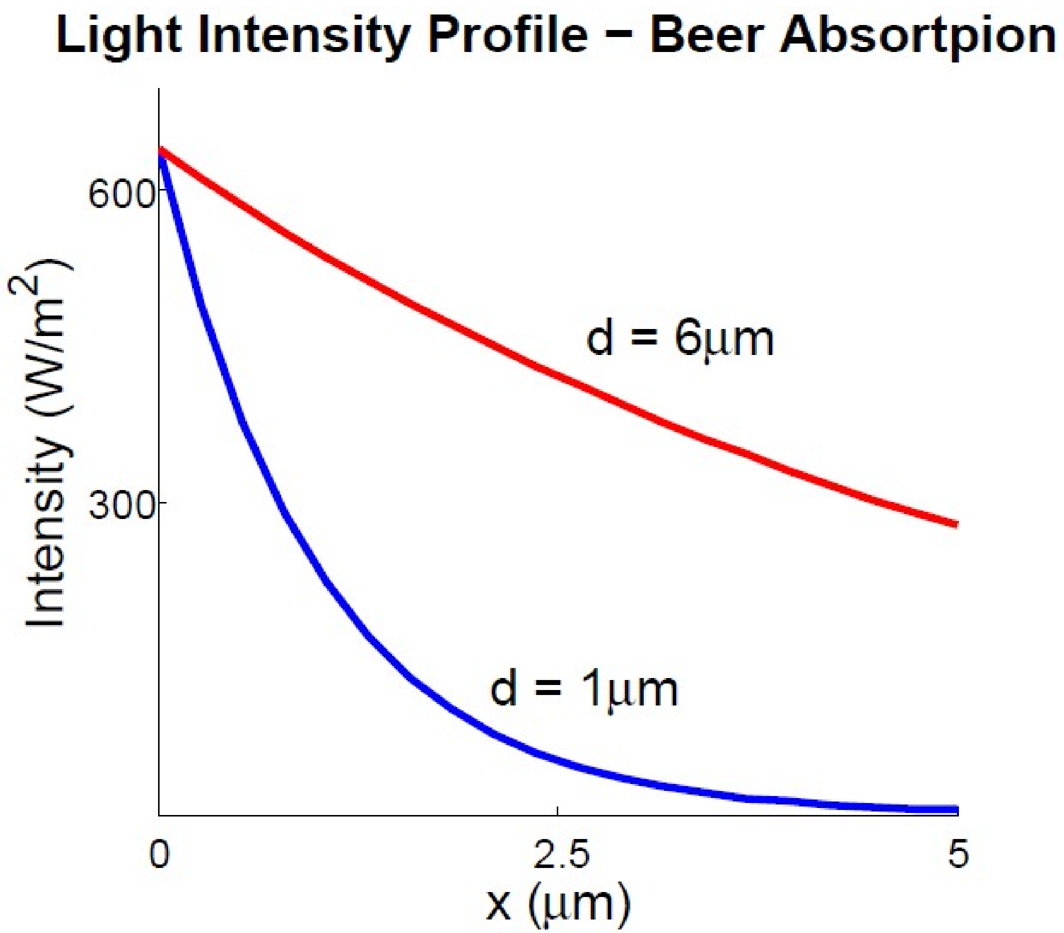


(van Oosten, 2009)

THEORY OF PHOTOBENDING

Beer-Lambert's law:

$$I(x) = I_0 e^{\left(-\frac{x\varphi}{d}\right)}$$



THEORY OF PHOTOBENDING

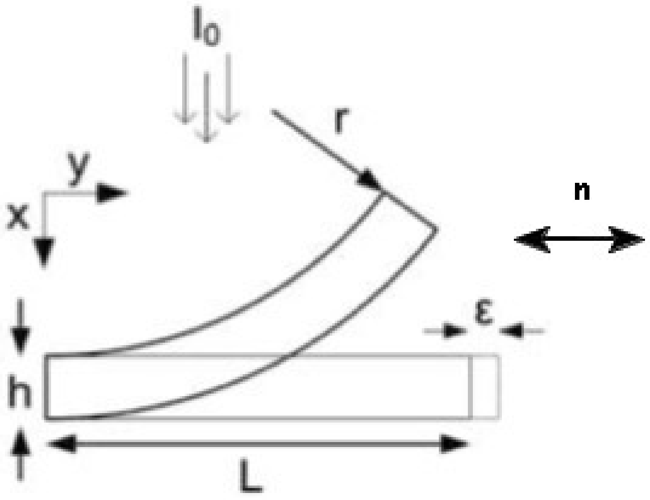
Deformation caused by light absorption:

$$\varepsilon_{light,y}(x) = \varphi P_{\parallel} I(x)cos^2\theta + \varphi P_{\perp} I(x)sin^2\theta$$

Photo-compliance correlates the absorbed light and the induced strain.

Resulting stress:

$$\sigma_y = \frac{\varepsilon_{bending} - \varepsilon_{light,y}}{(C_{11}sin^2\theta + C_{22}cos^2\theta)}$$



Bending radius:

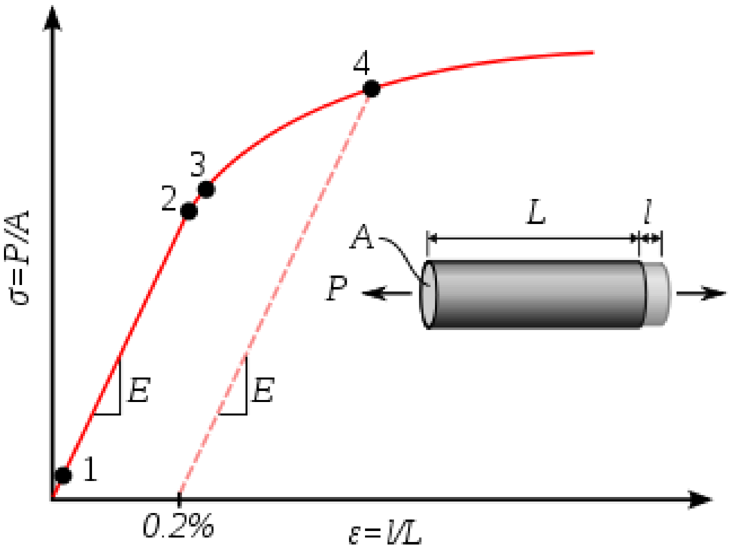
$$r = \frac{\varphi x^3}{6I_0Pd(-2d + 2de^{-\frac{\varphi x}{d}} + \varphi x + \varphi xe^{-\frac{\varphi x}{d}})}$$

HYPERELASTIC MATERIALS

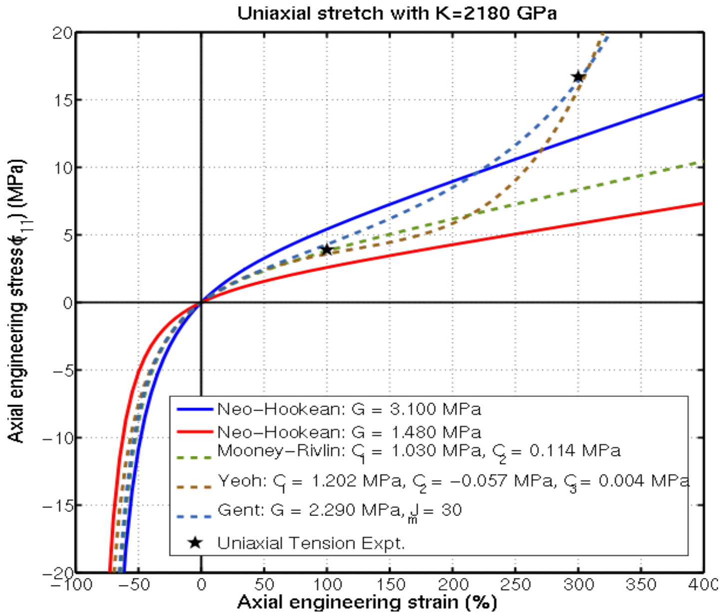
Strain energy density (incompressible version):

$$W = \frac{1}{2}\mu(\hat{I}_1 - 3) + \frac{1}{2}k(J_{el} - 1)^2$$

J_{el} depends on the photo-induced deformation.

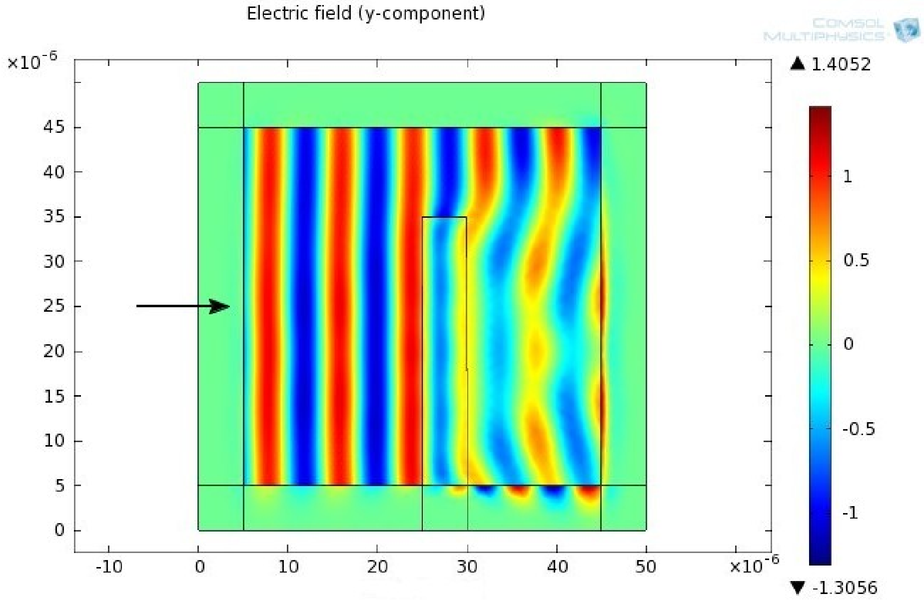


Linear elastic (Sigmund)



Hyperelastic (Bbanerje)

SIMULATION CONSTANTS

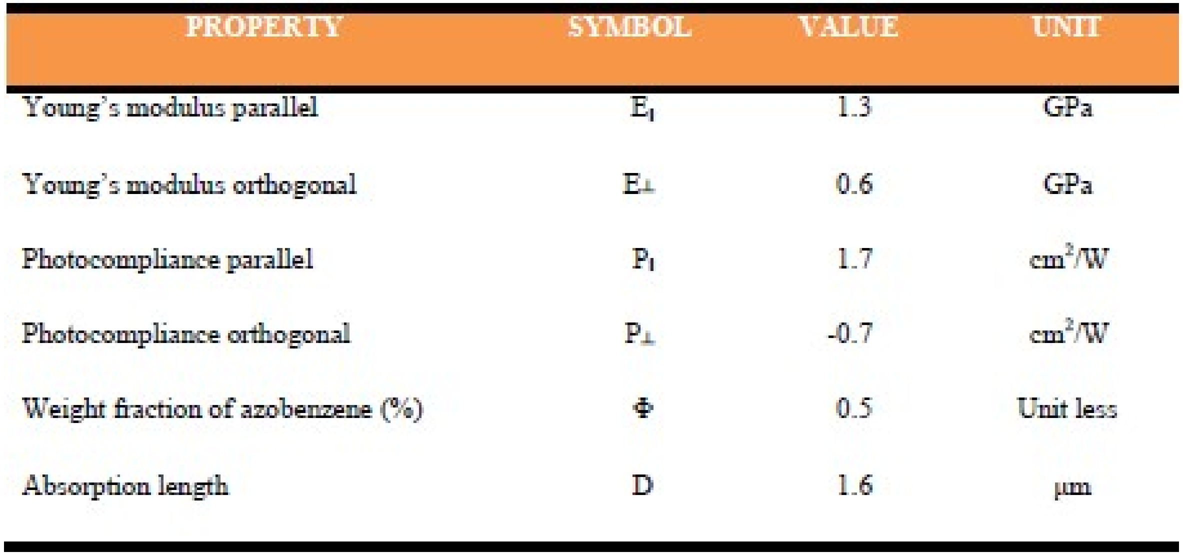


Characteristics common to each simulated case:

-Geometry

-Material properties

-Propagation direction of the electric field

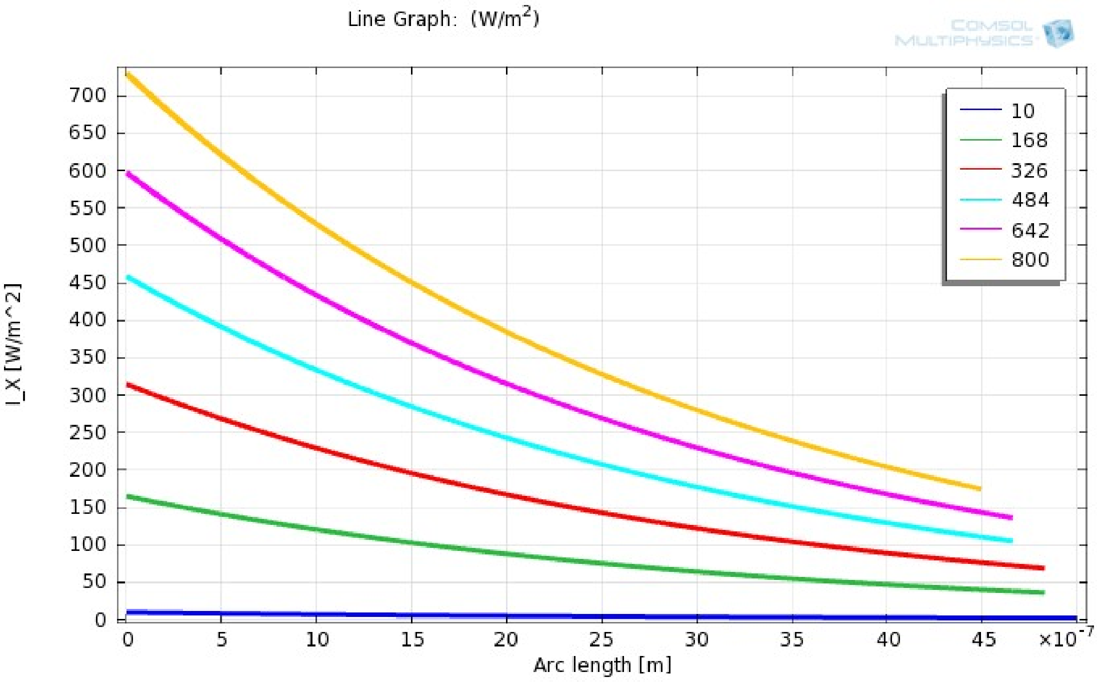


PROPERTY	SYMBOL	VALUE	UNIT
Young's modulus parallel	$E_\parallel$	1.3	GPa
Young's modulus orthogonal	$E_\perp$	0.6	GPa
Photocompliance parallel	$P_\parallel$	1.7	cm^2/W
Photocompliance orthogonal	$P_\perp$	-0.7	cm^2/W
Weight fraction of azobenzene (%)	Φ	0.5	Unit less
Absorption length	D	1.6	μm

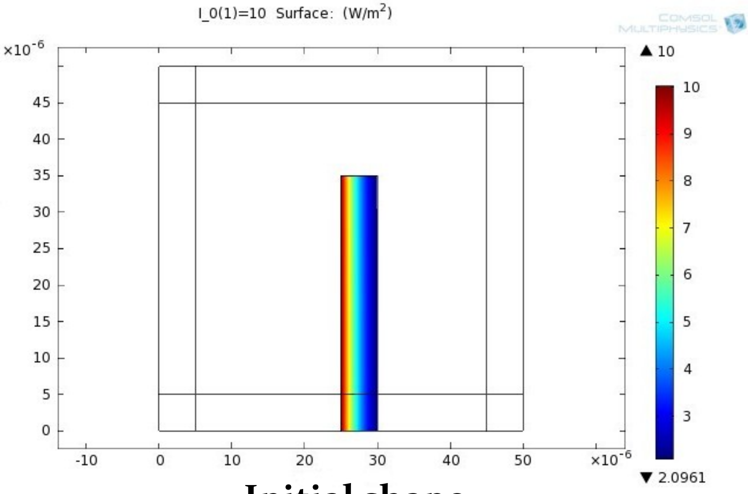
BEER-LAMBERT'S LAW OF ABSORPTION AND UNIAXIAL ALIGNMENT

Absorption law:

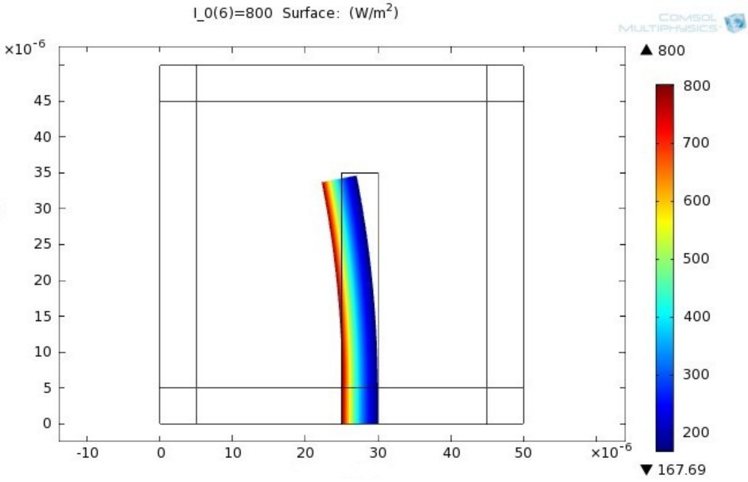
$$I(x) = I_0 e^{\left(-\frac{x\varphi}{d}\right)}$$



Intensity through the thickness of the sample

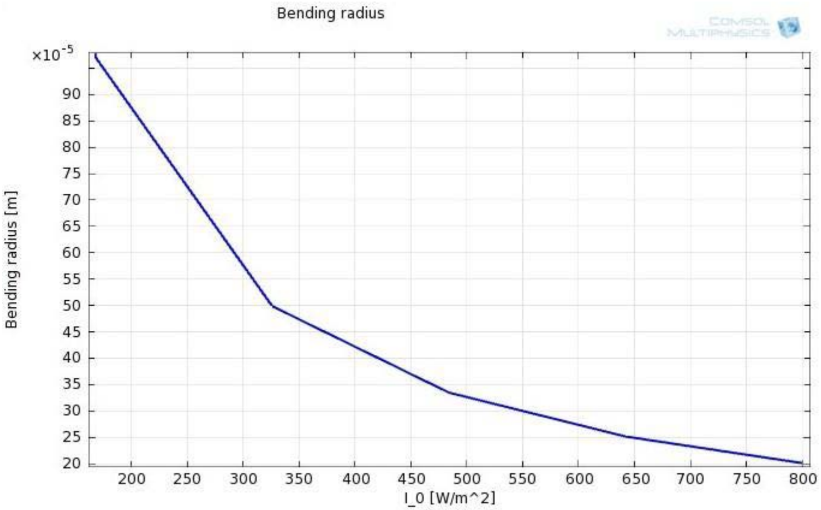


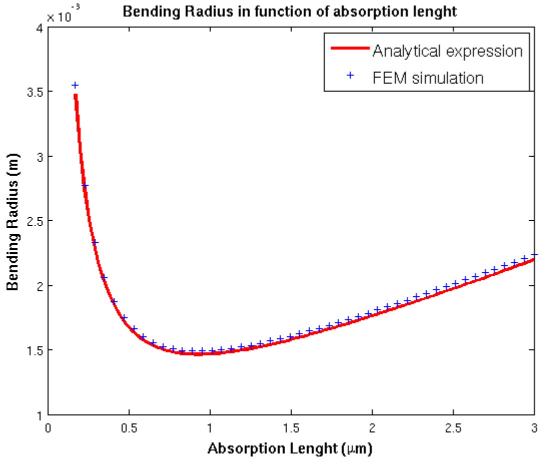
Initial shape

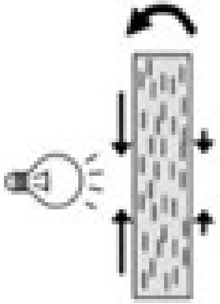


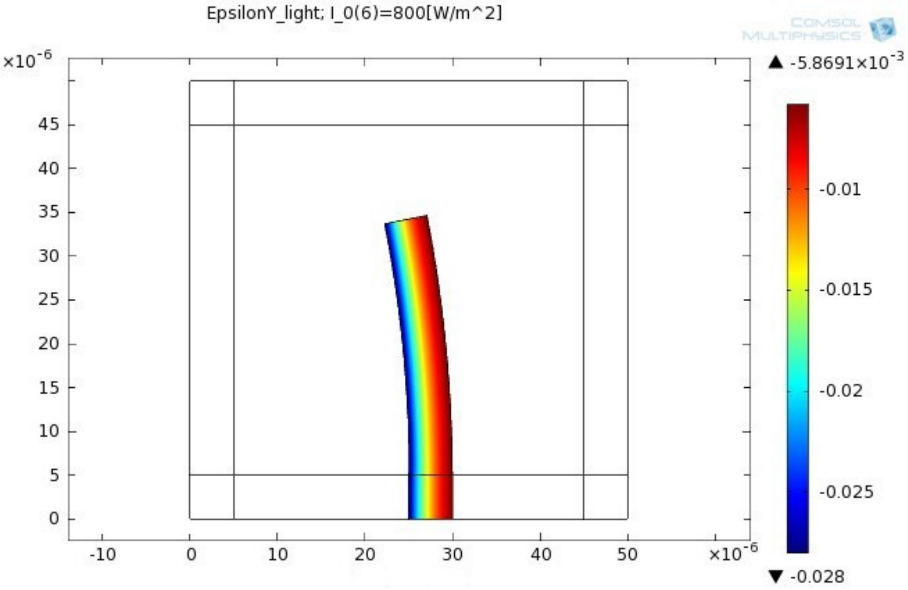
Final shape

BEER-LAMBERT’S LAW OF ABSORPTION AND UNIAXIAL ALIGNMENT


Bending radius

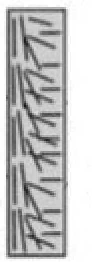

Bending Radius in function of absorption lenght

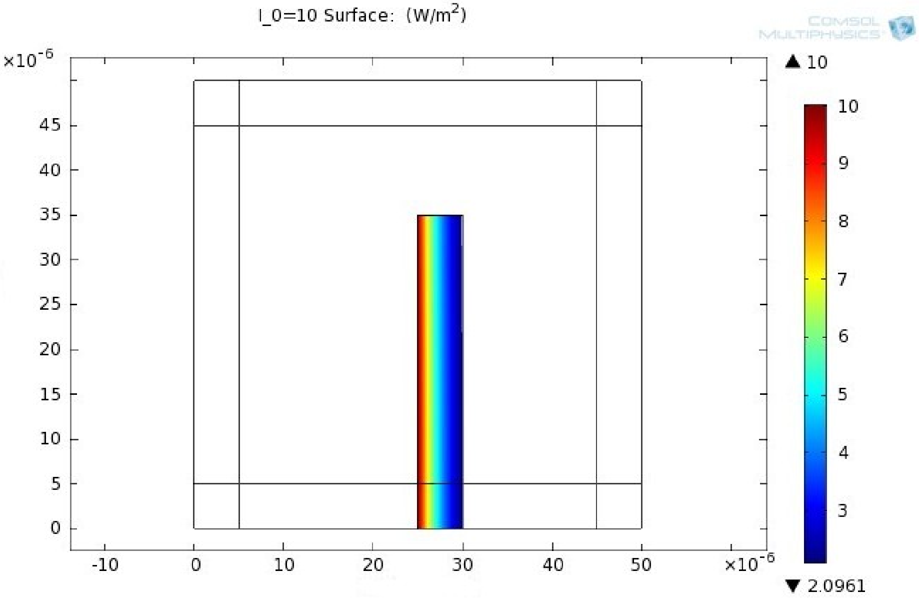



EpsilonY_light; I_0(6)=800[W/m^2]

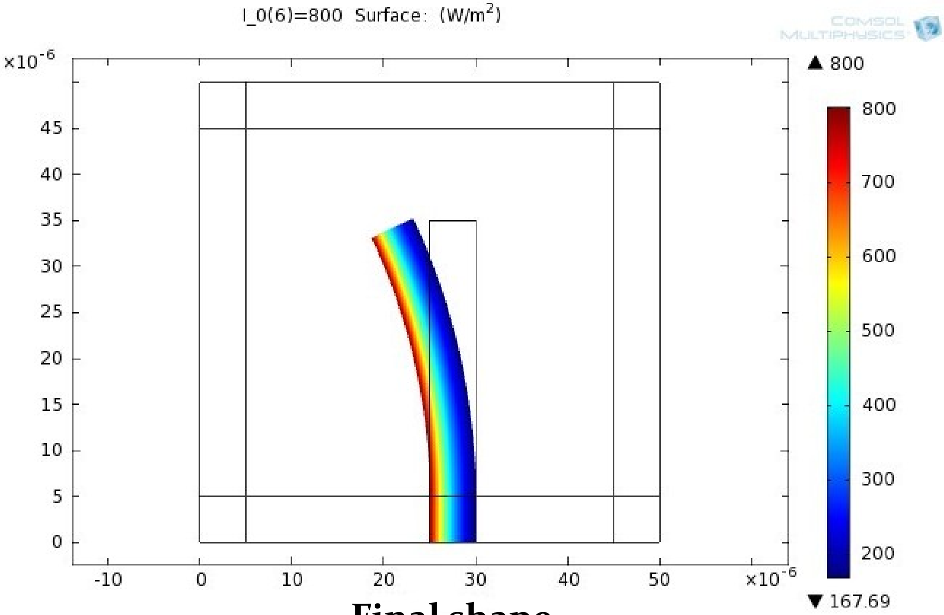
BEER-LAMBERT'S LAW OF ABSORPTION AND SPLAYED ALIGNMENT

Internal splayed alignment:



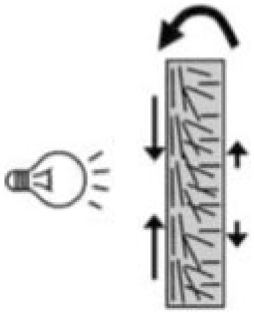


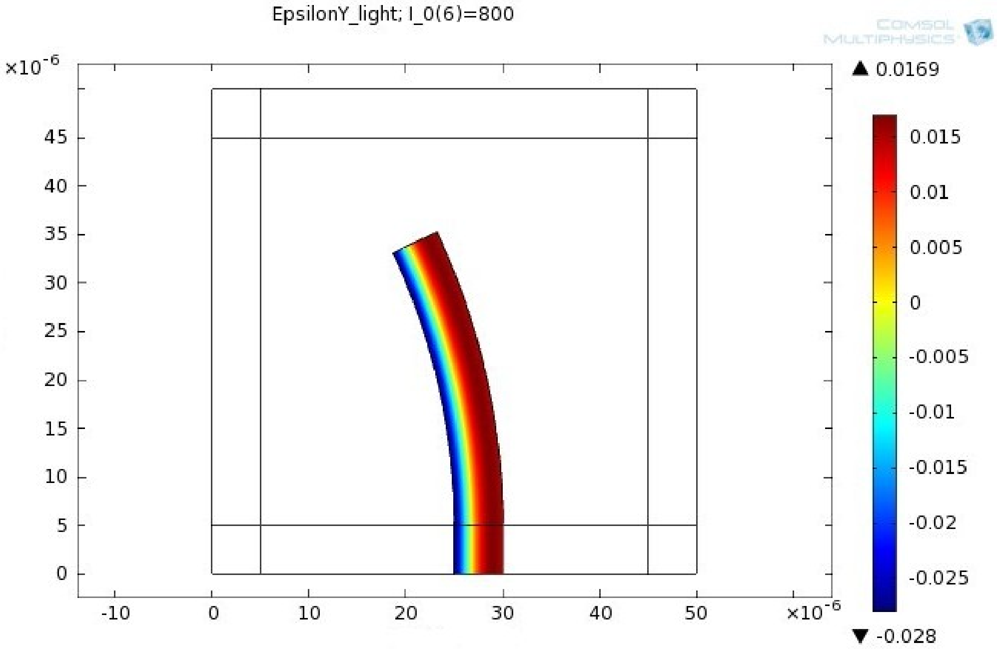
Initial shape

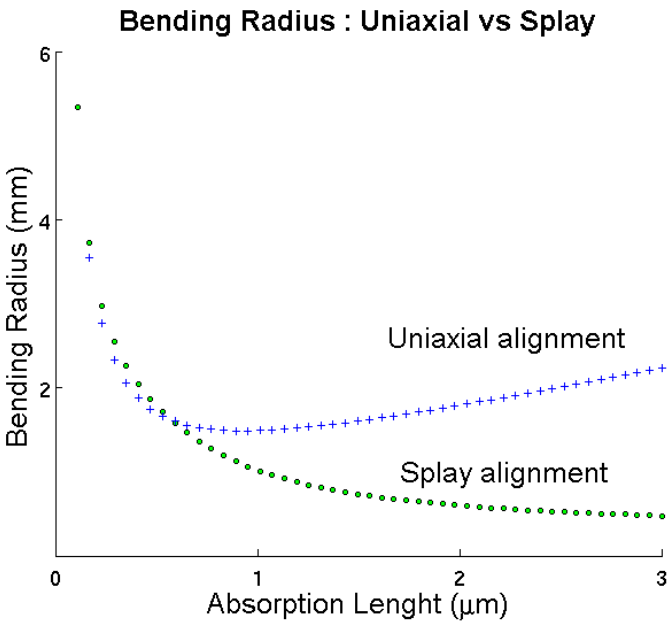


Final shape

BEER-LAMBERT'S LAW OF ABSORPTION AND SPLAYED ALIGNMENT

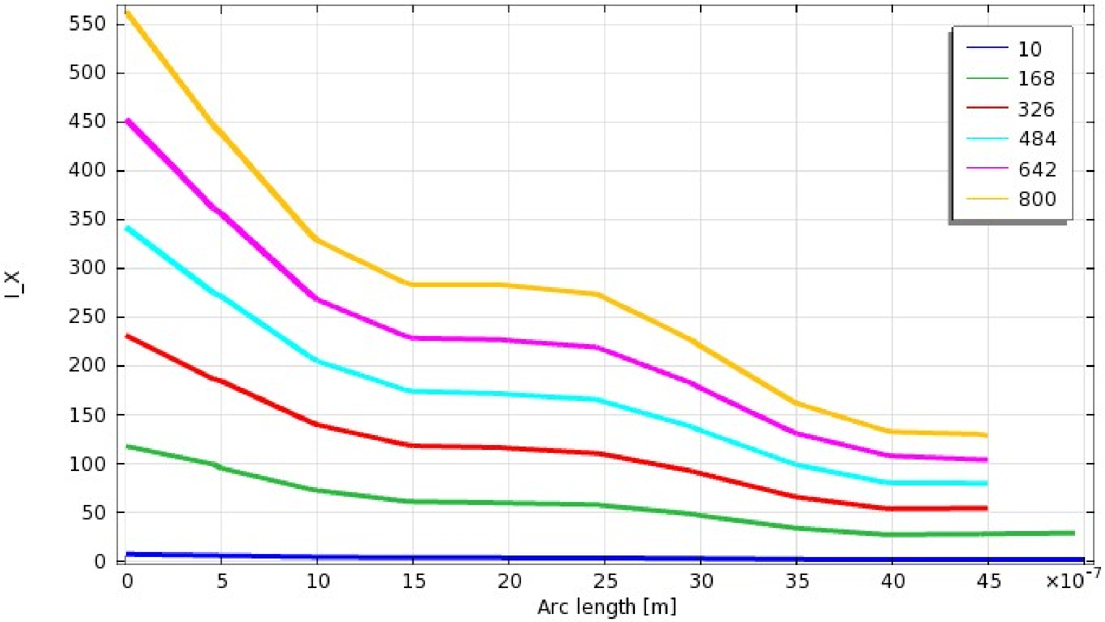




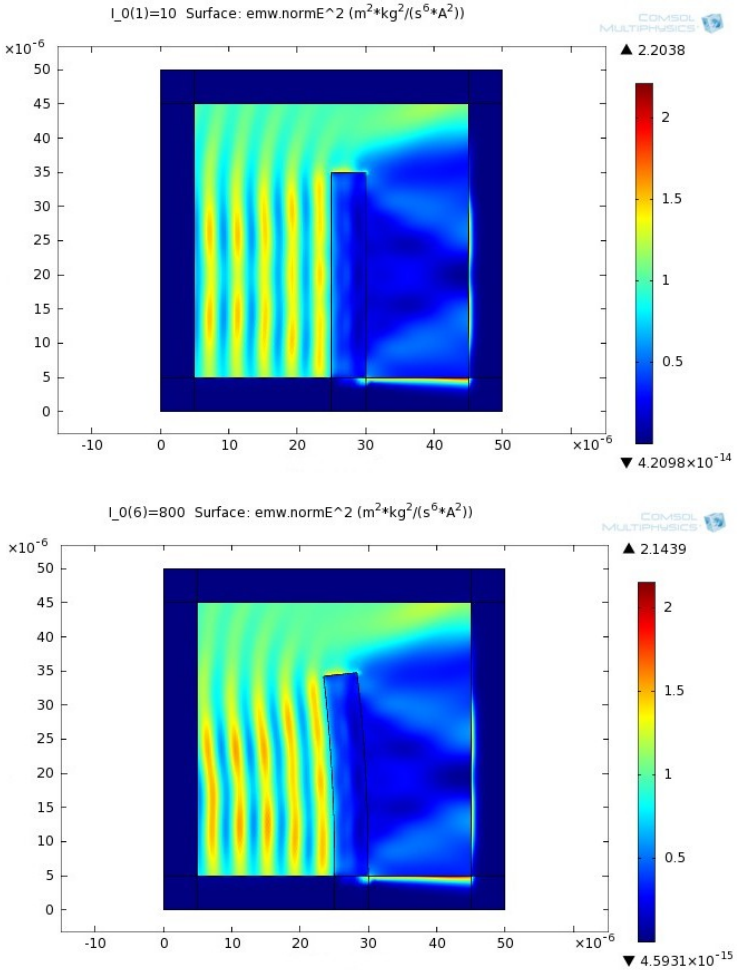


MAXWELL'S EQUATIONS AND UNIAXIAL ALIGNMENT

Absorption law: $$I(x) = C_0 \left|\left|E\right|\right|^2$$

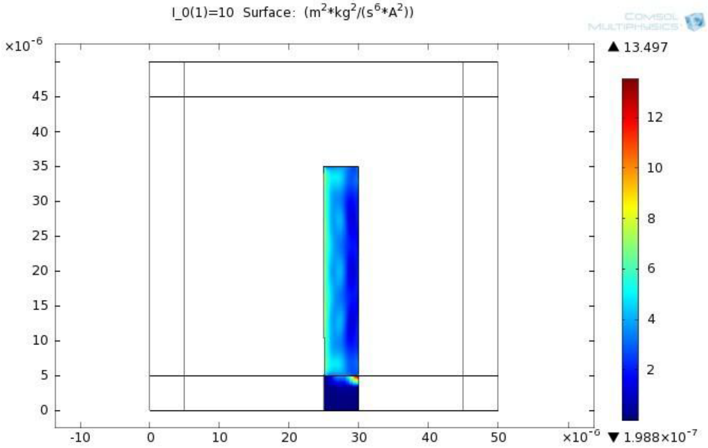


Intensity through the sample thickness

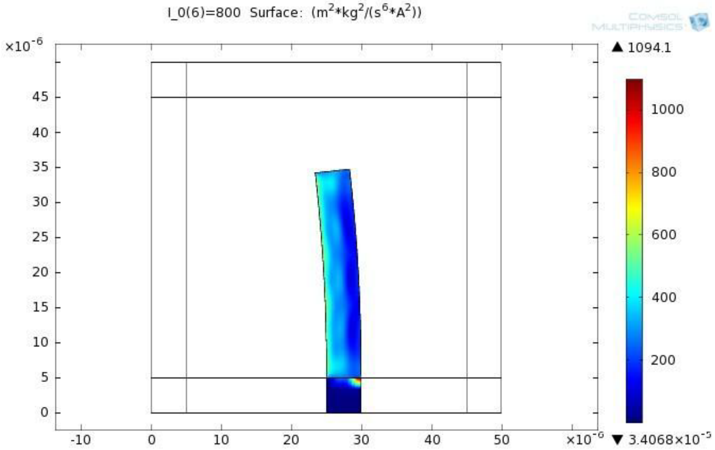


Variation of the squared norm

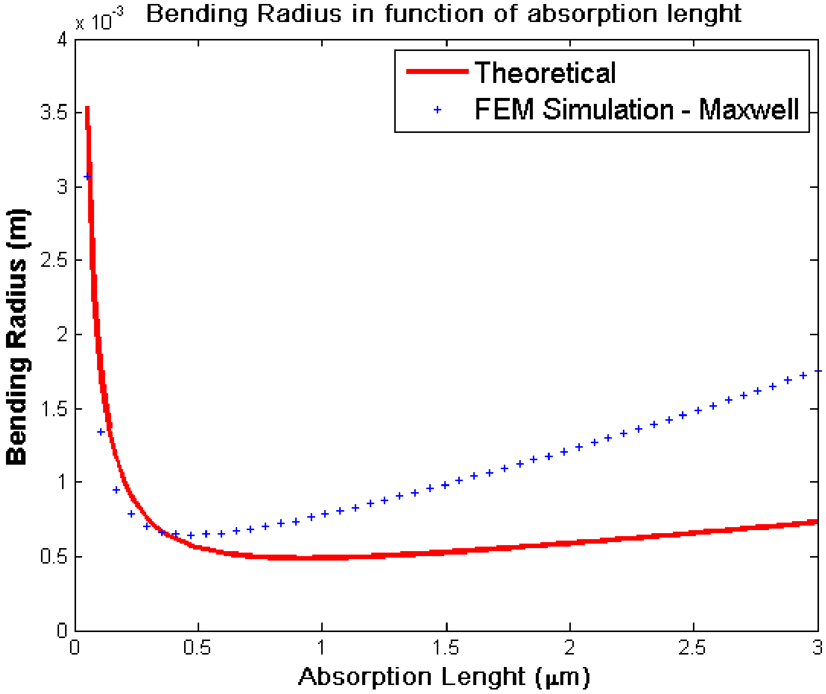
MAXWELL'S ABSORPTION LAW AND UNIAXIAL ALIGNMENT



Initial shape



Final shape

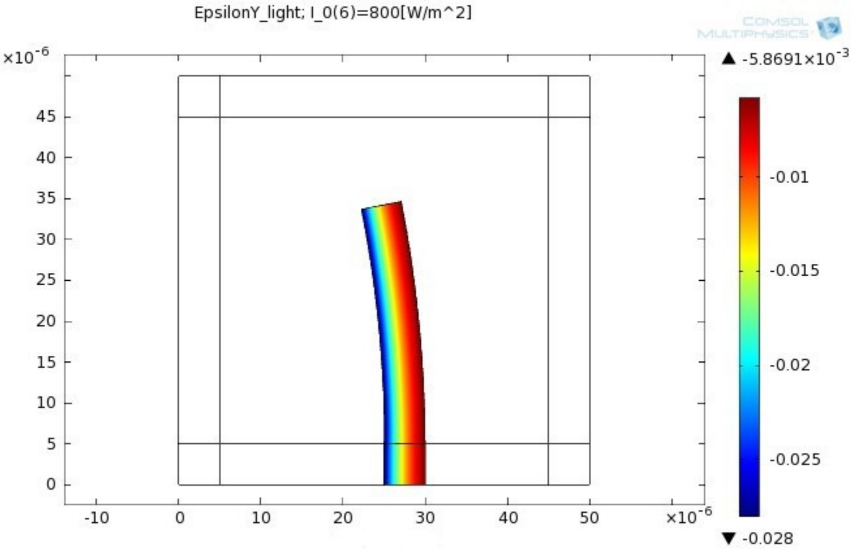


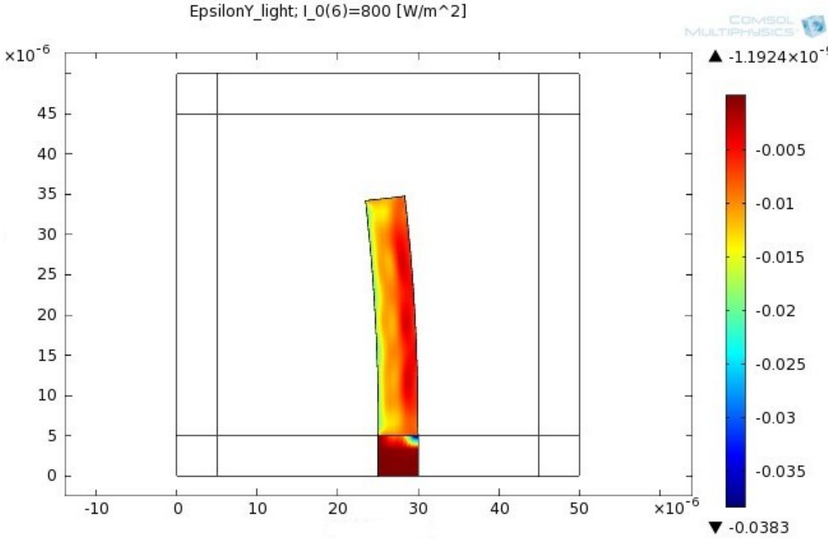
BEER-LAMBERT VS MAXWELL

Beer-Lambert

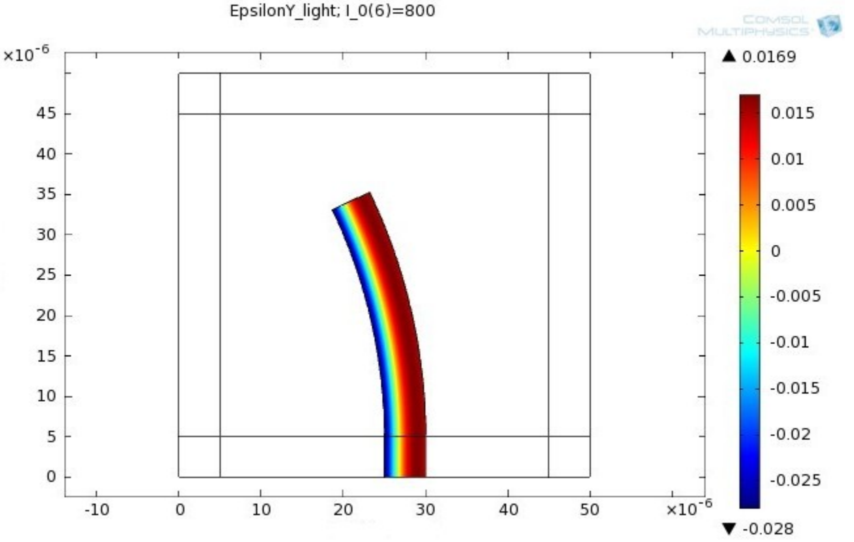
Maxwell

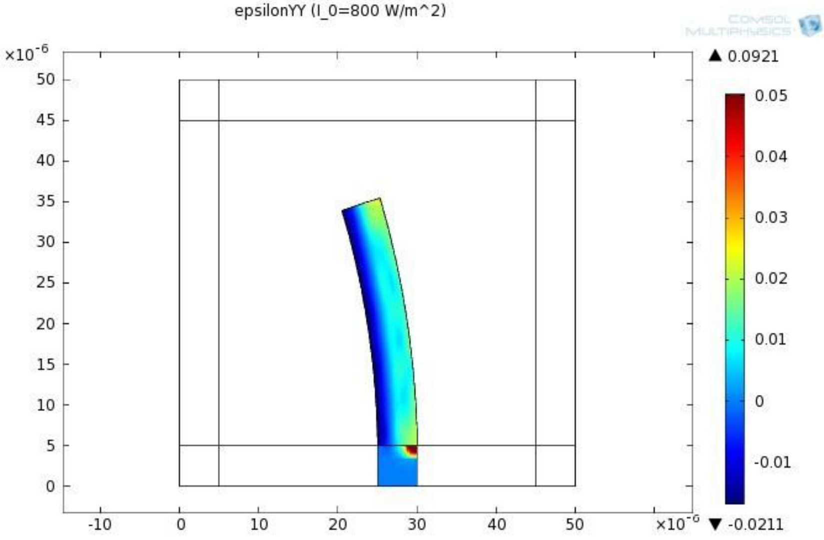
Uniaxial


EpsilonY_light; I_0(6)=800[W/m^2]


EpsilonY_light; I_0(6)=800 [W/m^2]

Splayed

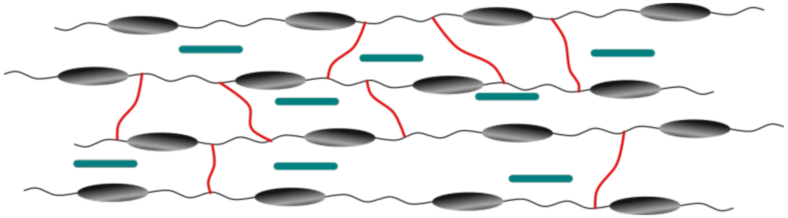

EpsilonY_light; I_0(6)=800

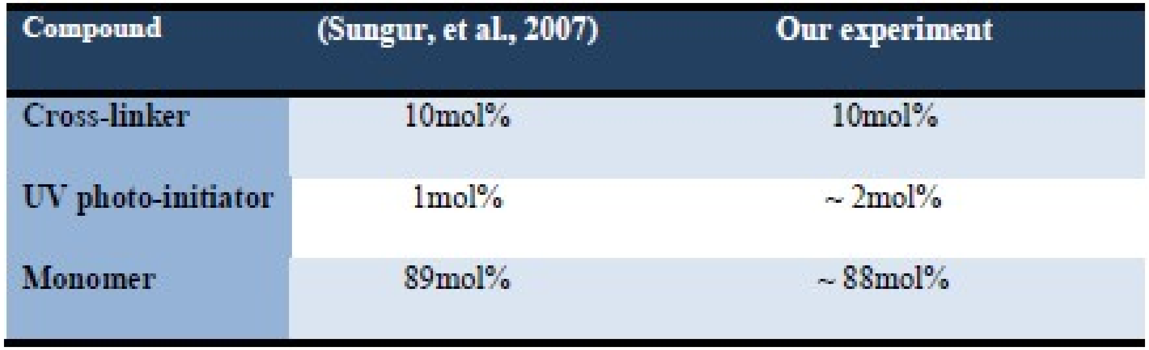

epsilonYY (I_0=800 W/m^2)

IMPLEMENTATION

STEPS

- Mixture into a coated glass cell.
- Heat to 90°C (liquid state).
- Cool down to 63°C (isotropic-nematic transition).
- Photo-polymerization with IR laser, hence solid structure.





Compound	(Sungur, et al., 2007)	Our experiment
Cross-linker	10mol%	10mol%
UV photo-initiator	1mol%	~ 2mol%
Monomer	89mol%	~ 88mol%

IMPLEMENTATION

WHAT WE DID

✓ 2D stationary simulations of LCE structures reacting to light stimuli, using two different approaches:

- Beer-Lambert's law
- Maxwell's equations

Applied to the internal configurations:

- Uniaxial
- Splayed

✓ Creation procedure by photo-polymerization of uniaxial aligned nematic LC monomers.

IN THE NEXT FUTURE

- ✓ Compare the theoretical and the experimental results.
- ✓ 2D time-dependent simulations.
- ✓ 3D stationary and time-dependent simulations.
- ✓ More complex shapes.

ACKNOWLEDGMENTS

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