7th International Meeting on

UNILATERAL PROBLEMS IN STRUCTURAL ANALYSIS

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A model for the mechanical response with damage of collagenous biostructures

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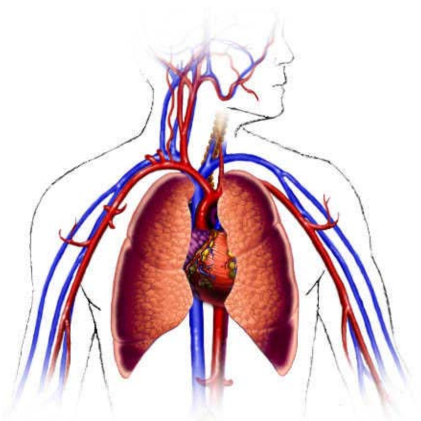
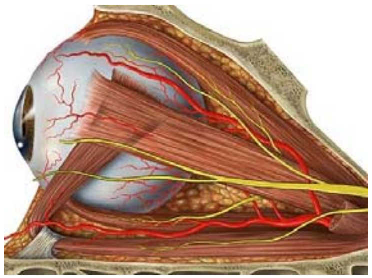
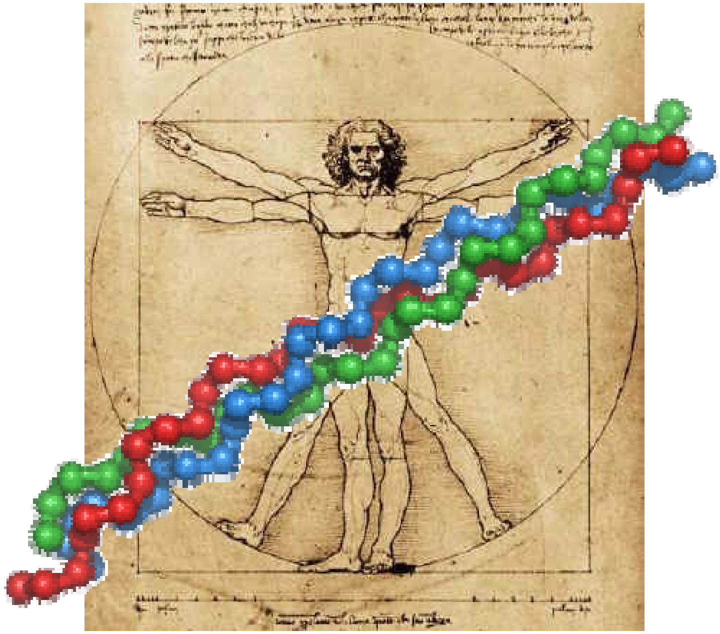
MOTIVATION

Collagen is the most abundant protein of the human body

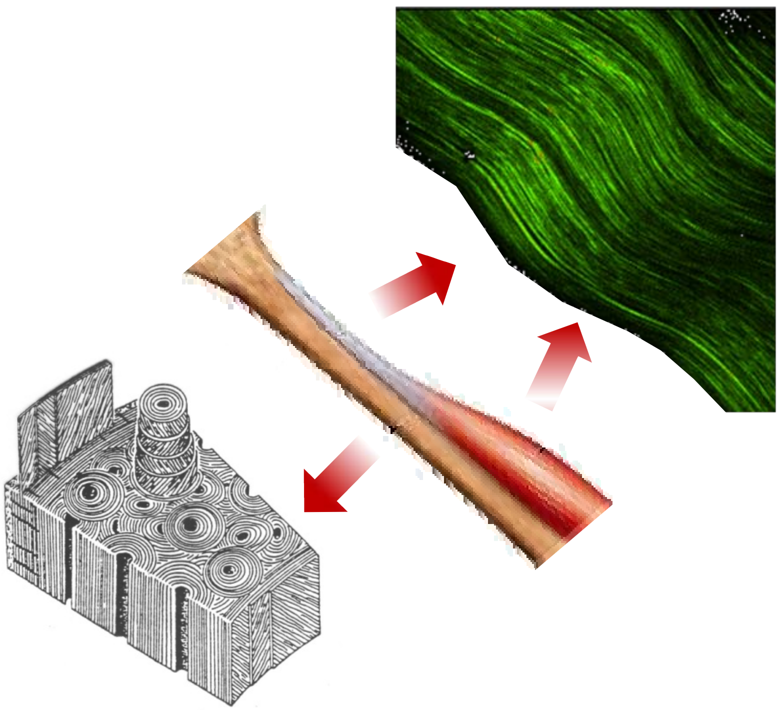


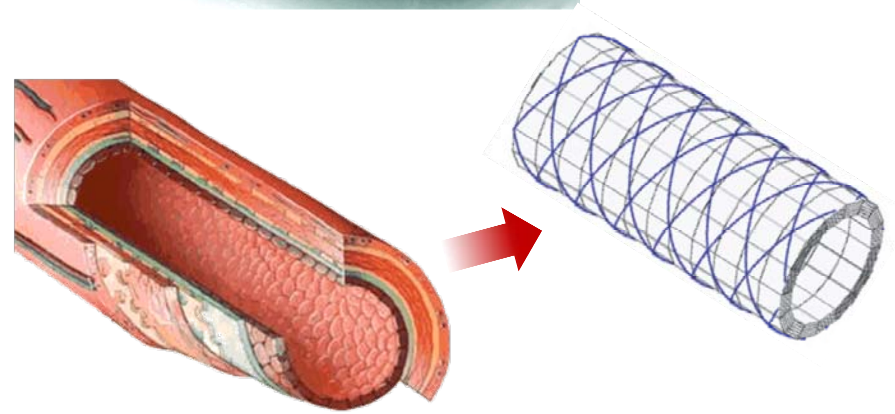




MOTIVATION

Collagen organization reflects its key role in the mechanical strength and functionality of living tissue





Macro-, micro- and nano-scale characteristics of collagenous structures highly affect tissues mechanics

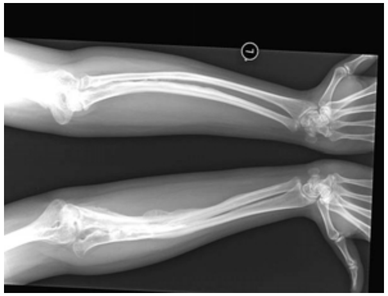
MOTIVATION: A Need for Mechanical Models

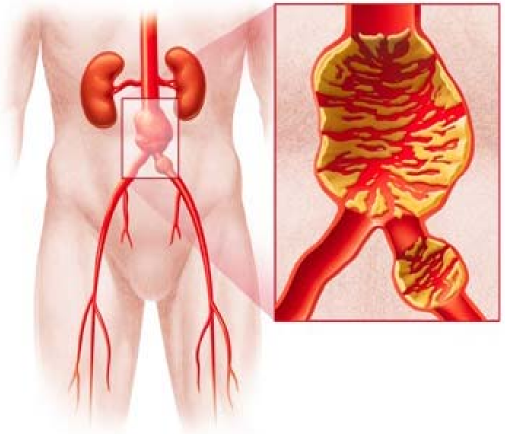
Multiscale Mechanical Modeling of Collagenous Tissues

At macroscale: mechanics of tissues affects organs functionality

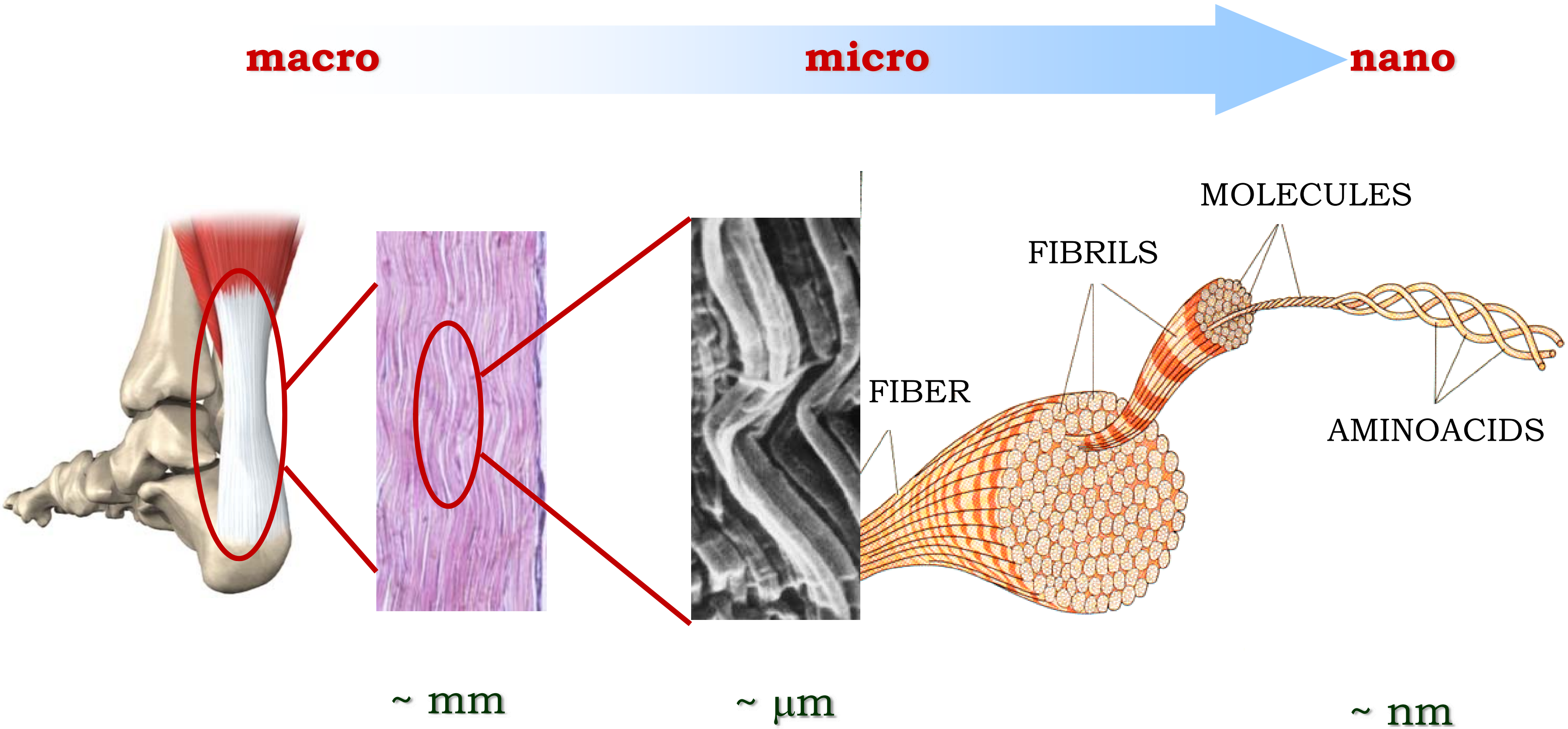
At microscale: Cellular stress environment affects molecular pathways leading to tissue remodeling

At nanoscale: Injuries, diseases and healing are often related with molecular alterations



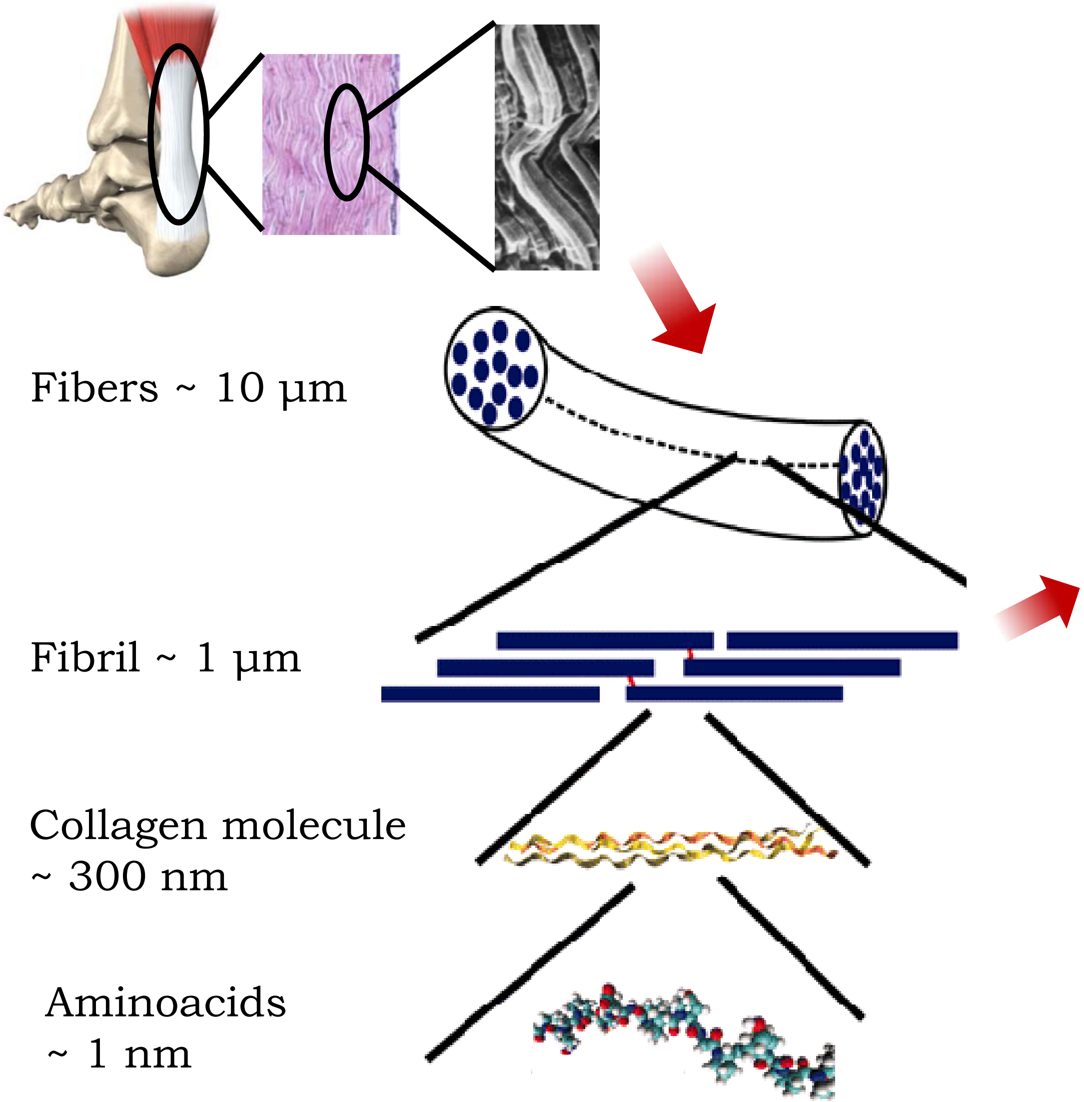


MOTIVATION

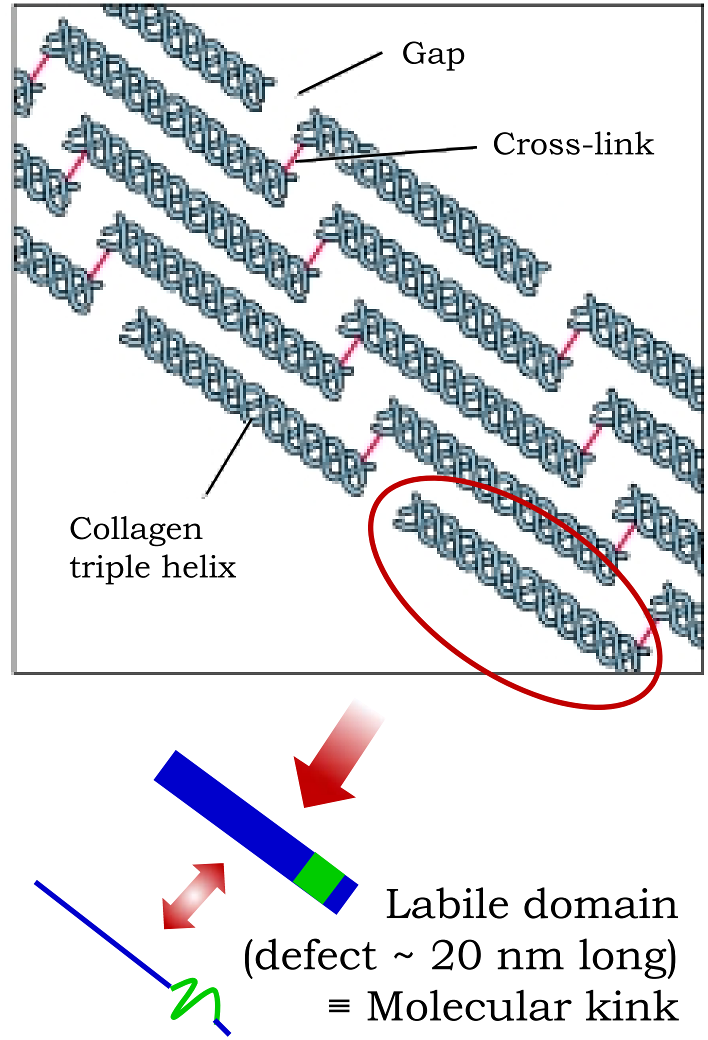


Organized hierarchical structure
from the nano- up to the macro-scale.

MOTIVATION



Fibers ~ 10 µm
Fibril ~ 1 µm
Collagen molecule
~ 300 nm
Aminoacids
~ 1 nm



Gap
Cross-link
Collagen
triple helix
Labile domain
(defect ~ 20 nm long)
≡ Molecular kink

OUTLINE

⇒ Mechanics of soft tissues: macroscale → nanoscale

⇒ A multiscale elasto-damaging model for collagenous fibrils:

- Nanoscale: Molecular model
- Nanoscale: Cross-links model
- Microscale: Fibril model

⇒ Conclusions and Perspective: Back to the macroscale

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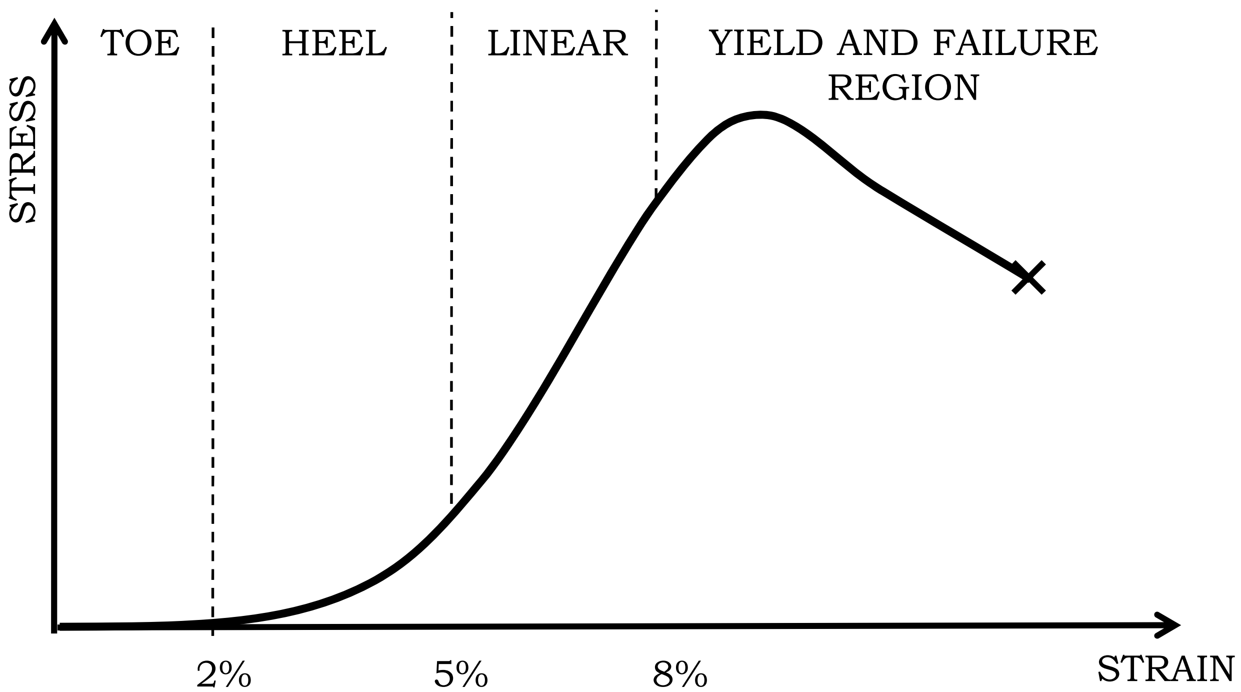
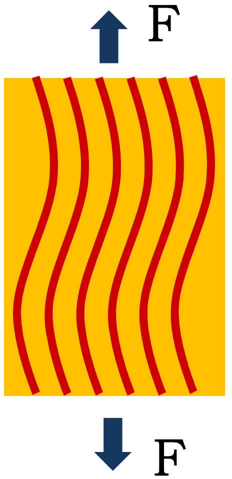
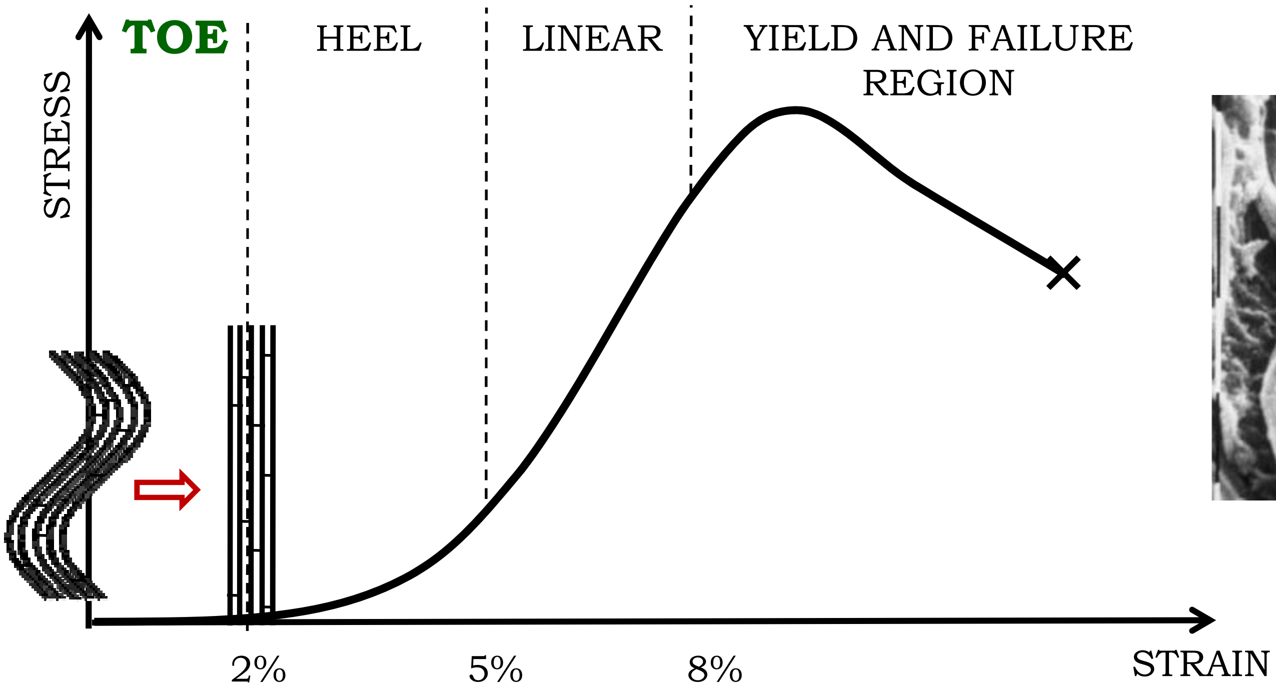
Macroscale response is ruled by
micro- and nano-scale mechanisms

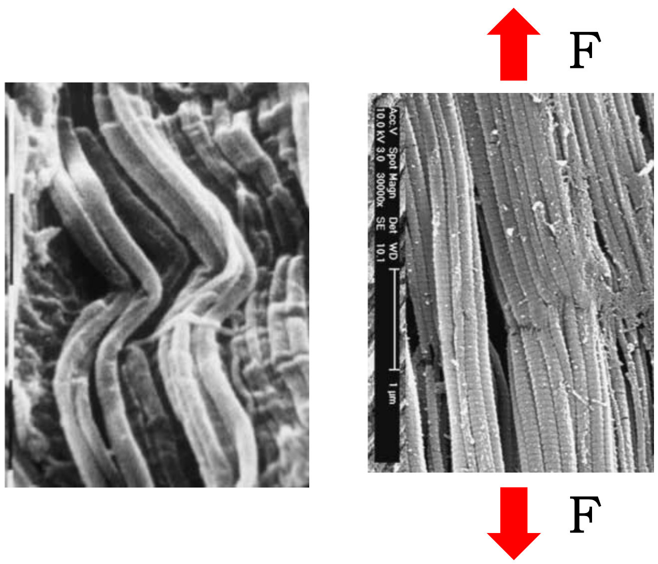




TOE REGION:

removal of the fibers/fibrils microscopic crimps

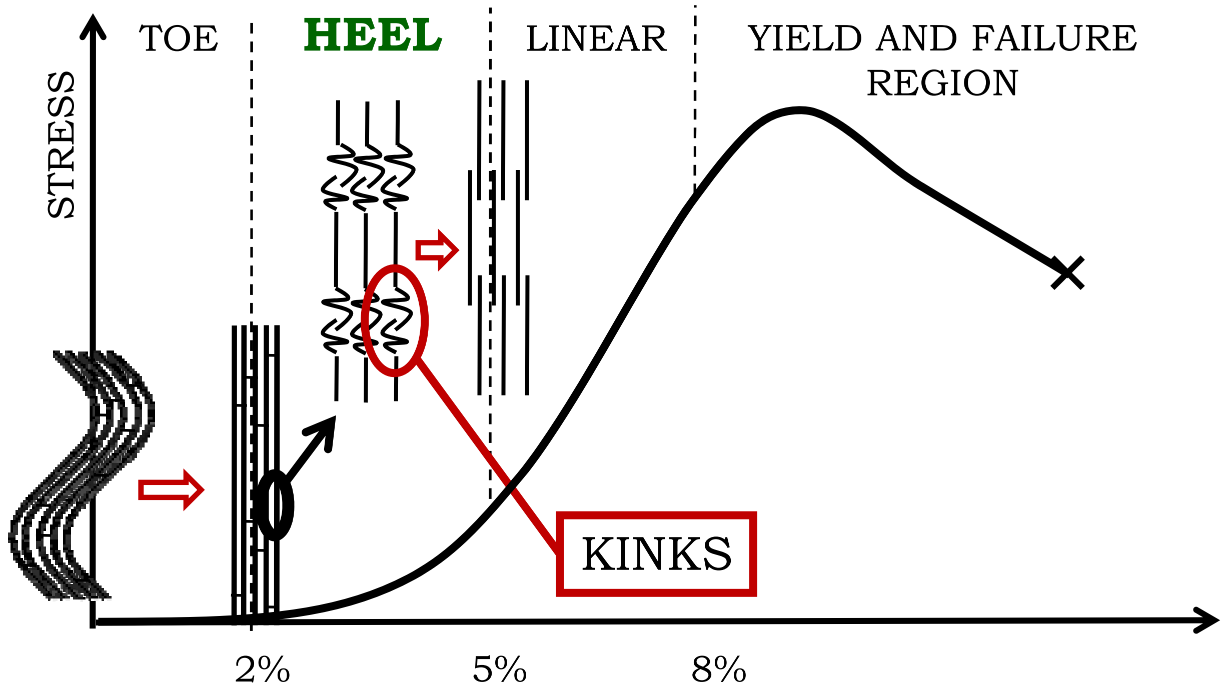




Fratzl (1997), Freed (2006)

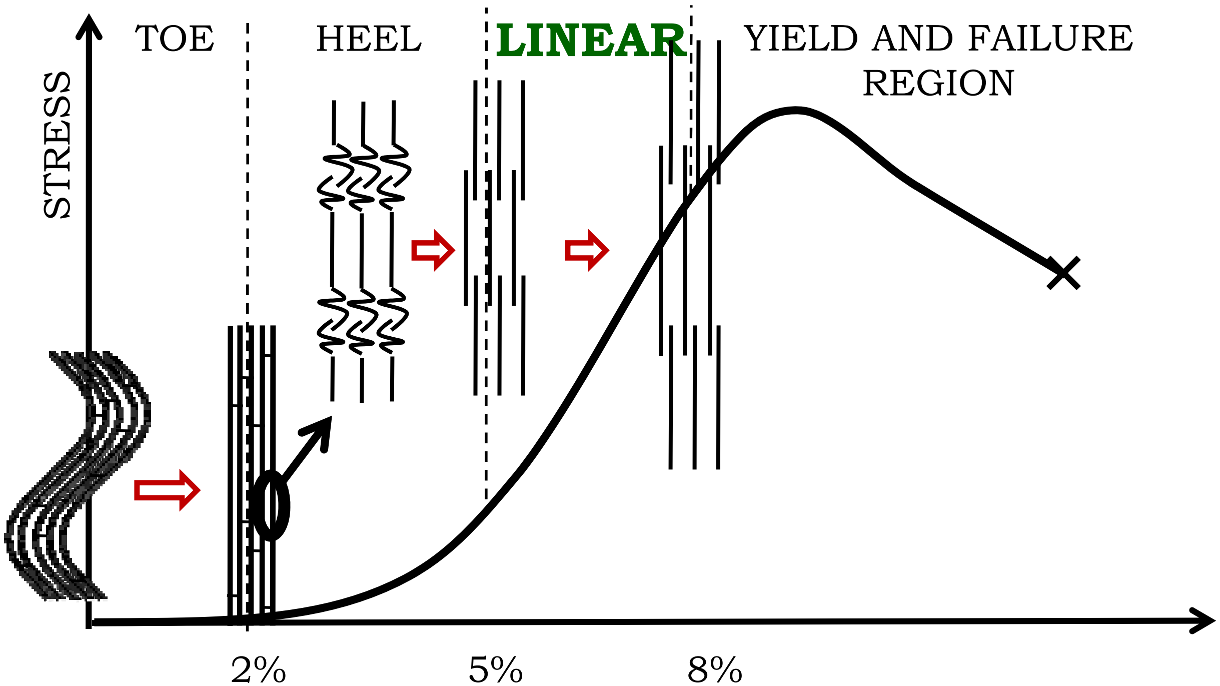
HEEL REGION:

kinks straightening due to entropic mechanisms



Sasaki (1996), Fratzl (1997)

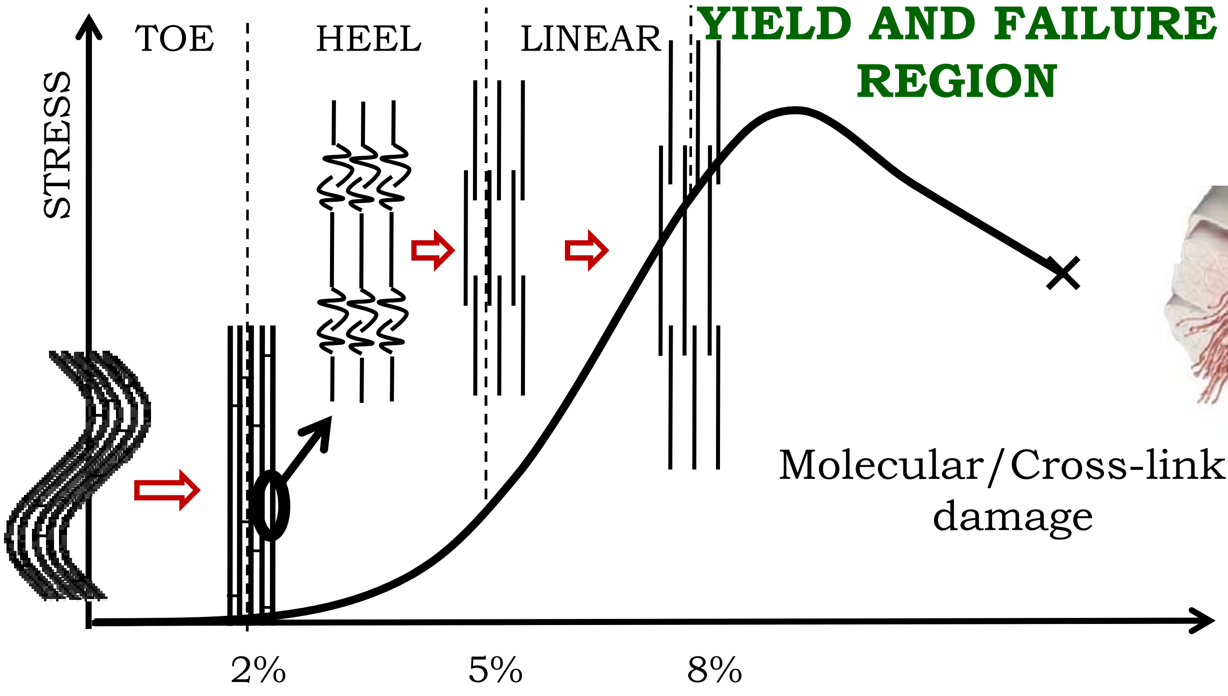
LINEAR REGION:
stretching of collagen triple-helices



Fratzl (1997), Buehler (2007)

YIELD AND FAILURE REGION:

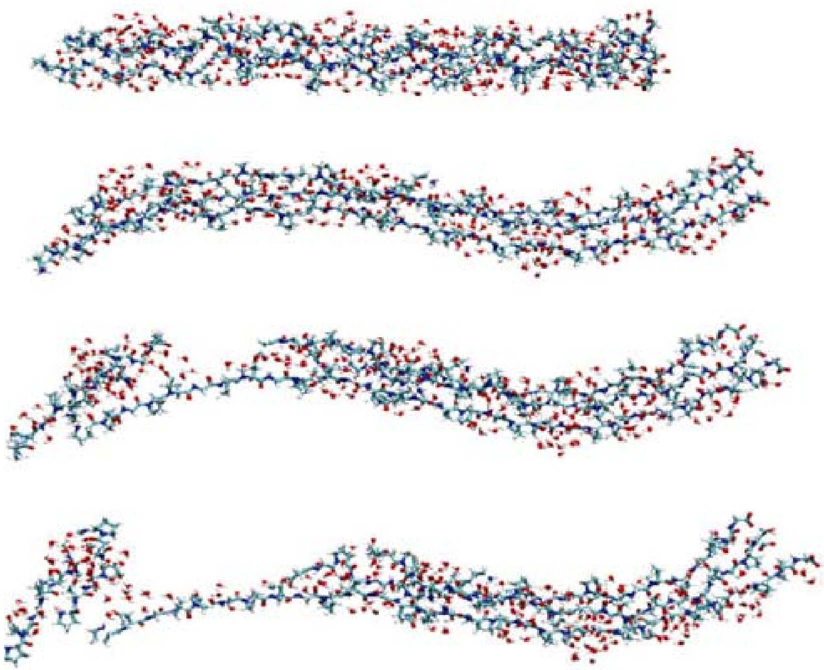
Nanoscale mechanisms



Molecular/Cross-links damage

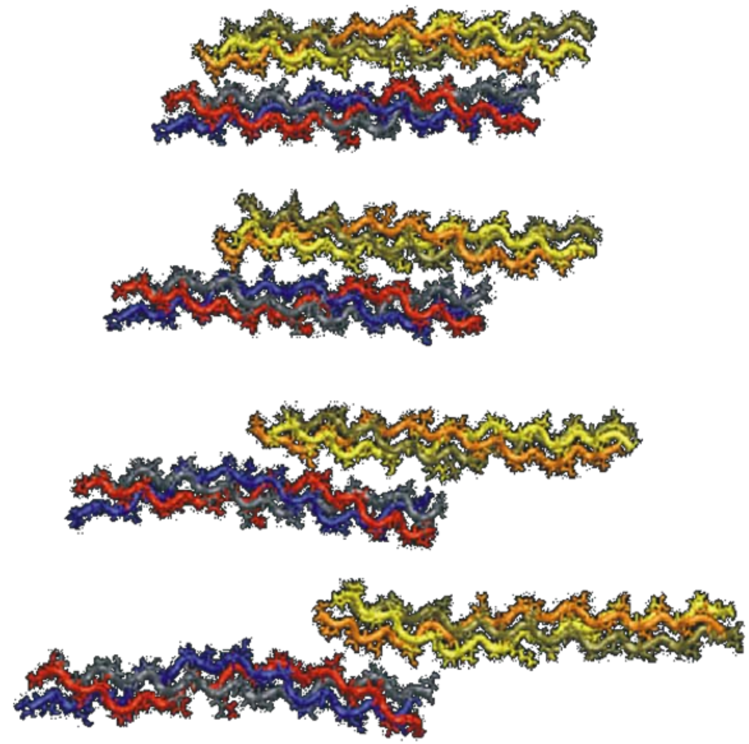
YIELD AND FAILURE REGION:

Molecular crack:



Damage

Molecular slippage
due to cross-link damage:



Buehler (2008)

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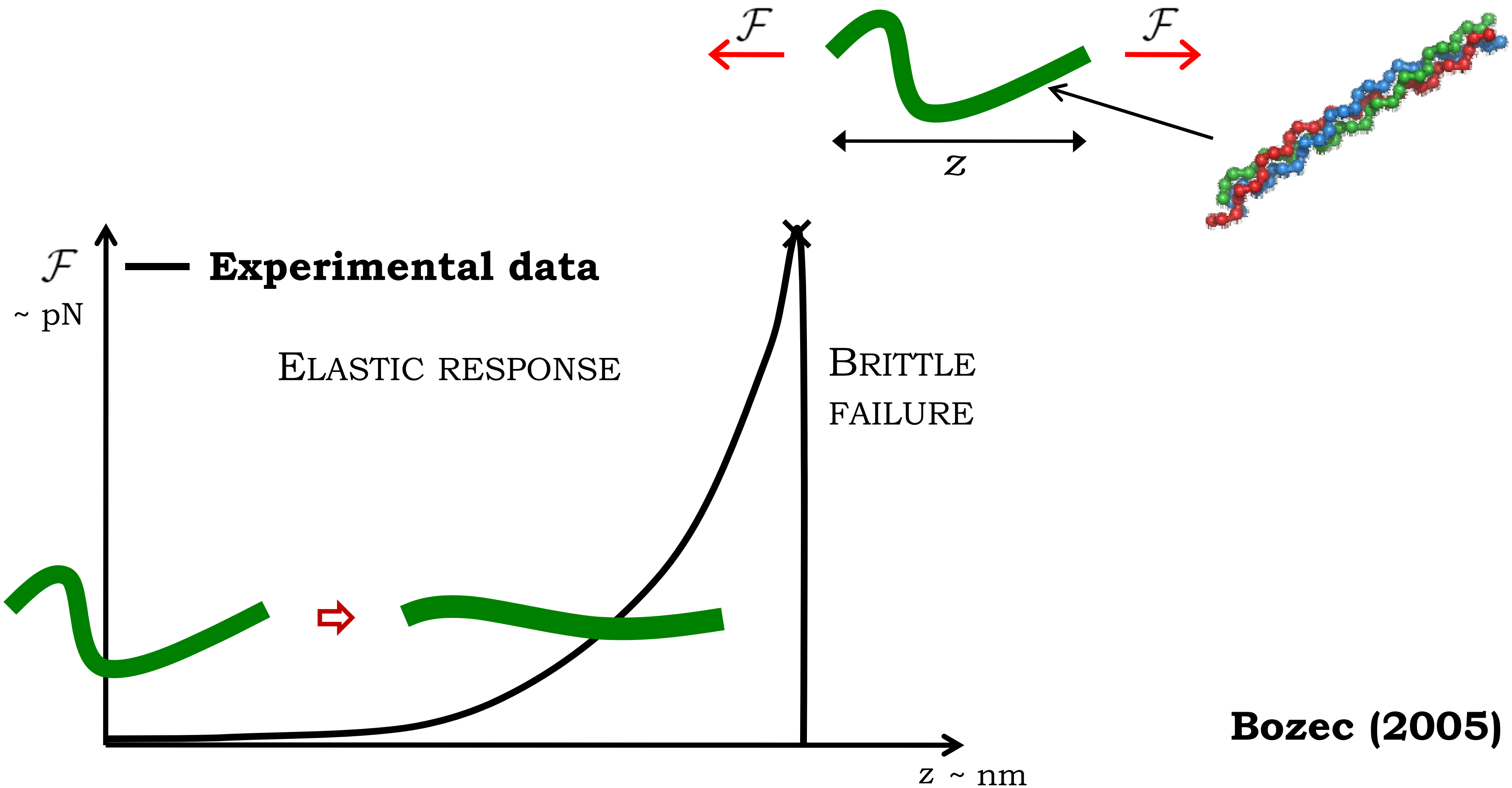
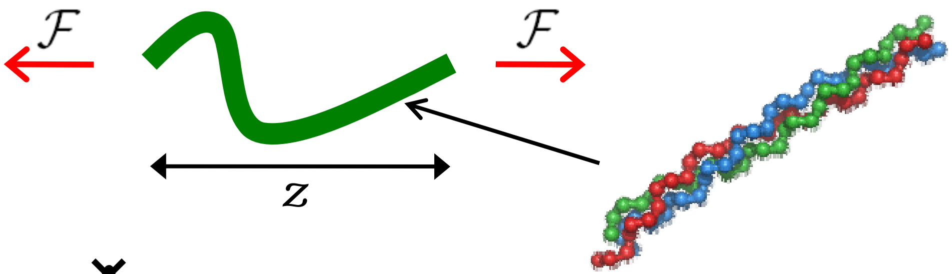
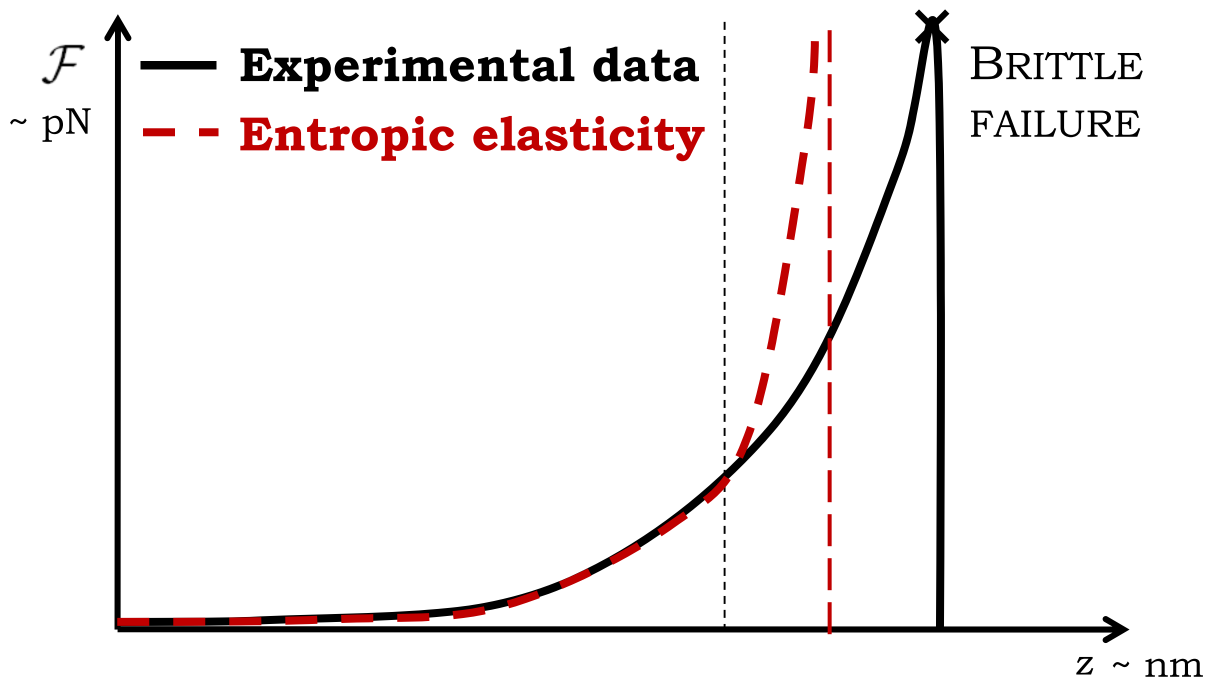
Atomic Force Microscopy of an isolated molecule:



Bozec (2005)

Atomic Force Microscopy of an isolated molecule:





Bozec (2005)
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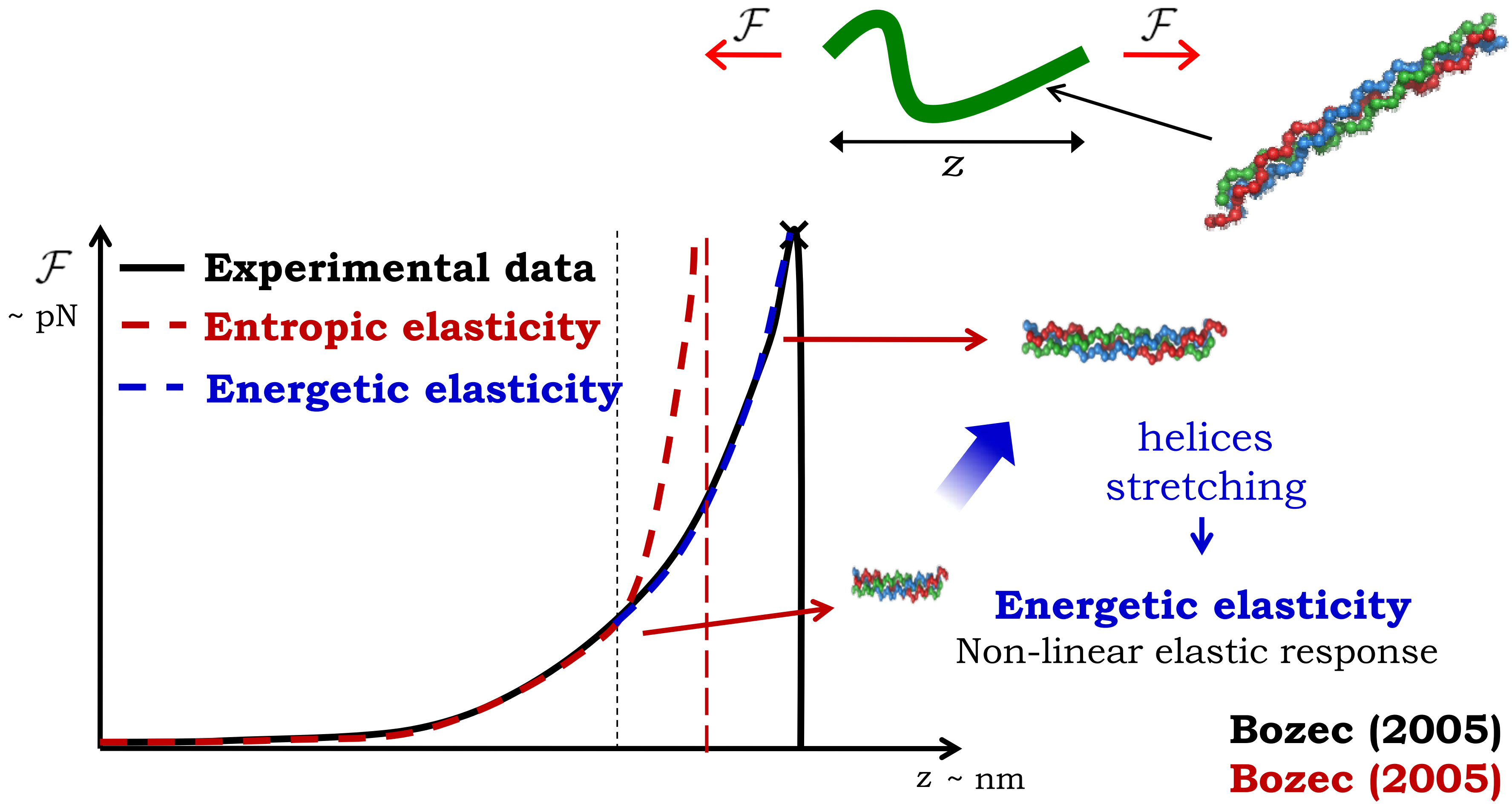
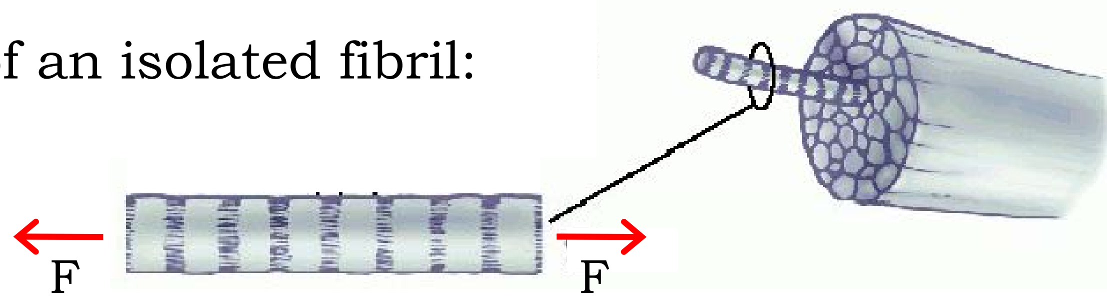
Atomic Force Microscopy of an isolated molecule:

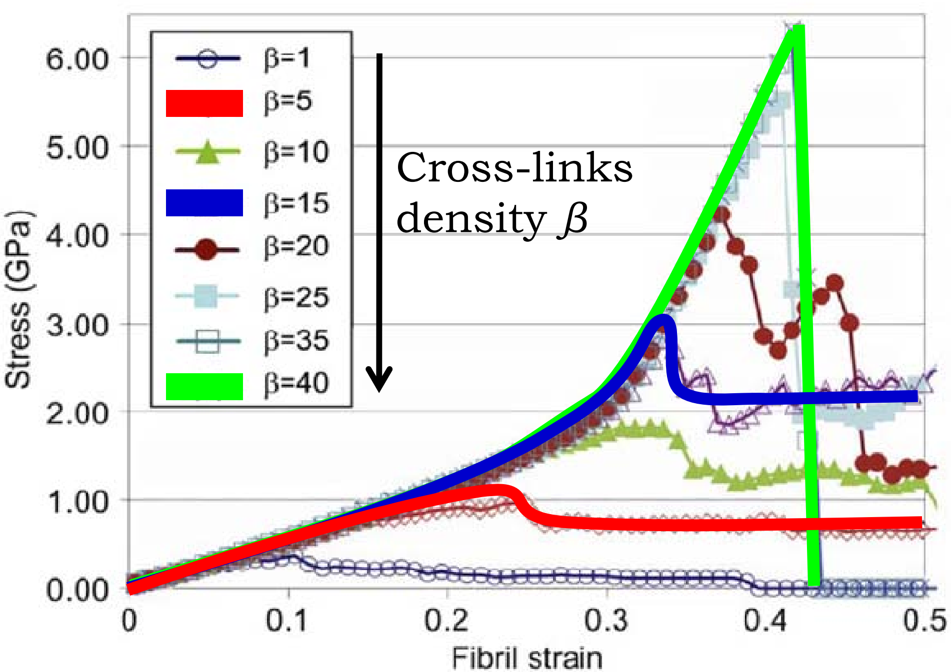


Bozec (2005)
Bozec (2005)
Maceri et al. (2010)

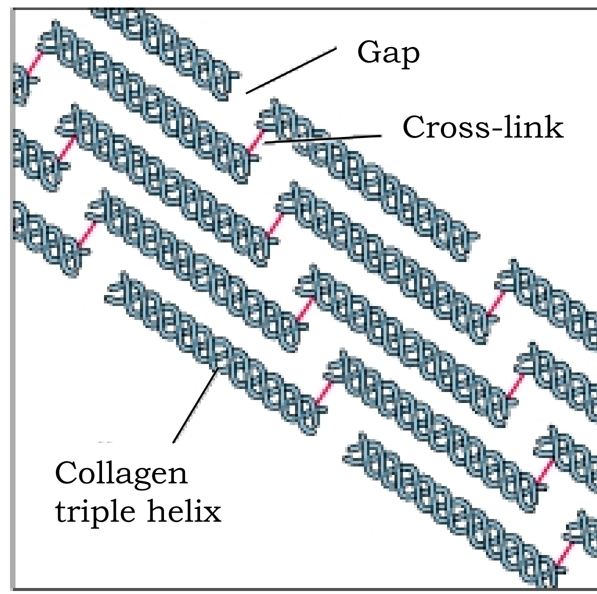
Homogeneous traction of an isolated fibril:

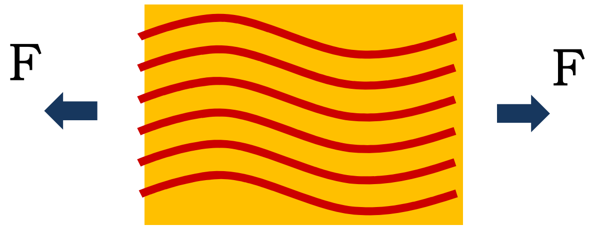


Dynamical molecular simulations:
(Buehler, 2008)



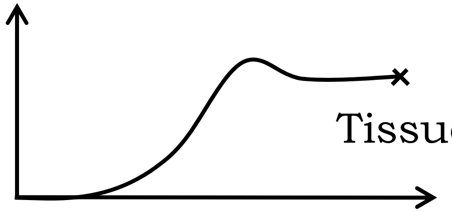
$\beta \approx 15 \rightarrow 1$ covalent cross-link/molecule



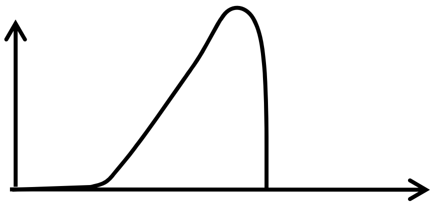


NUMBER OF CROSS-LINKS

Reduced stiffness and ductile mechanisms



Increased strength and brittle-like behaviour



Fibrils elasto-damaging mechanical behaviour affects the overall tissue response *in corpore*.

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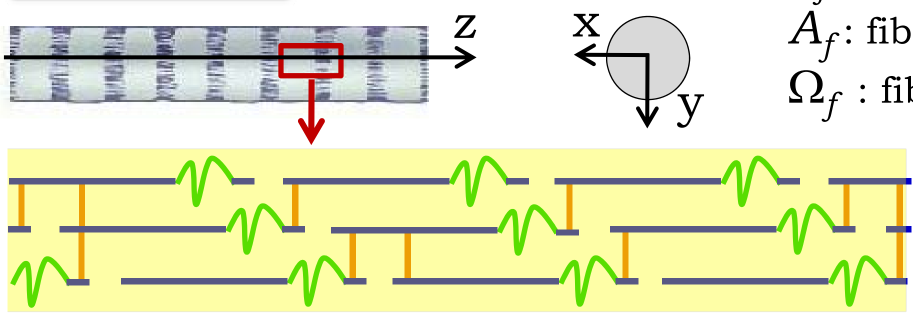
Geometry



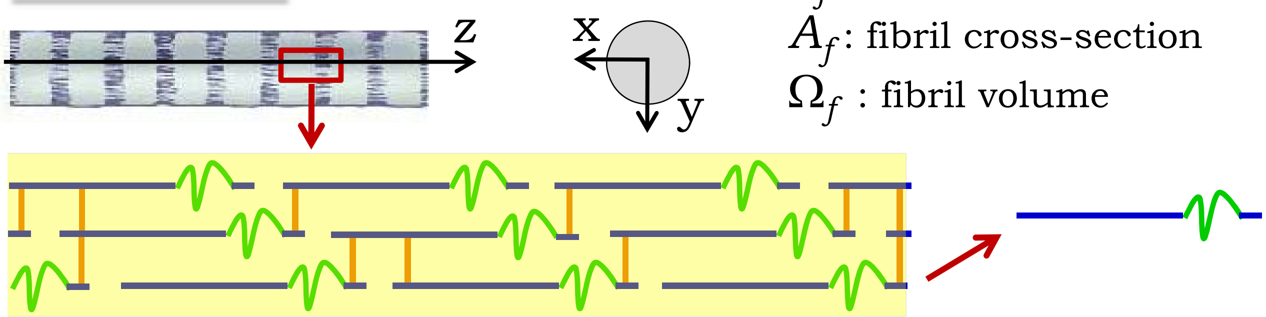
L_f : fibril length

A_f: fibril cross-section

Ω_f : fibril volume

A Model for Collagenous Fibrils

Geometry



L_f : fibril length
A_f: fibril cross-section
Ω_f : fibril volume

N_m: number of molecules
L_m : molecular length
A_m: molecular cross-section
Ω_m : molecular volume

Number of molecules

$$\hat{\mu} = \frac{\text{void}}{\text{solid}} + 1$$

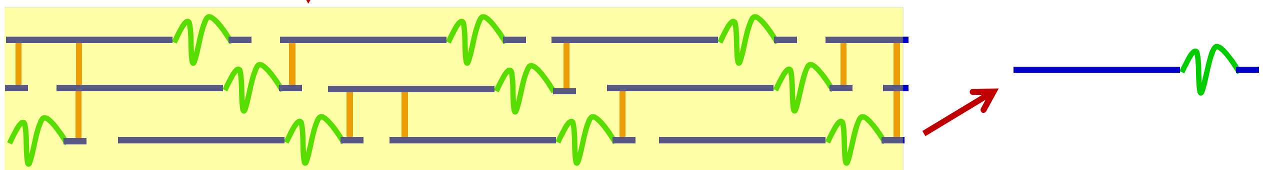
along fibril length $\hat{n}_s(x,y) = \dfrac{L_f}{\hat{\mu}_s(x,y) L_m}$

on fibril cross-section $\hat{n}_p(z) = \dfrac{A_f}{\hat{\mu}_p(z) A_m}$

Averaged quantities: $\mu_s, \; \mu_p, \; n_s, \; n_p$

$$N_m = n_s n_p \qquad \Omega_f = \mu_p \mu_s N_m \Omega_m = \mu N_m \Omega_m$$

Geometry

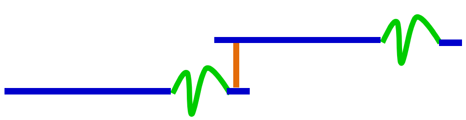


L_f : fibril length
A_f: fibril cross-section
Ω_f : fibril volume

N_m: number of molecules
L_m : molecular length
A_m: molecular cross-section
Ω_m : molecular volume

N_{cl}: number of cross-links → Expressed in terms of molecular number:

$$\hat{n}_{cl}(z) = \hat{\lambda}_p(z)\hat{n}_p(z)$$



$$N_{cl} = \int_{L_f} \hat{n}_{cl}(z)\, dz = \lambda N_m$$

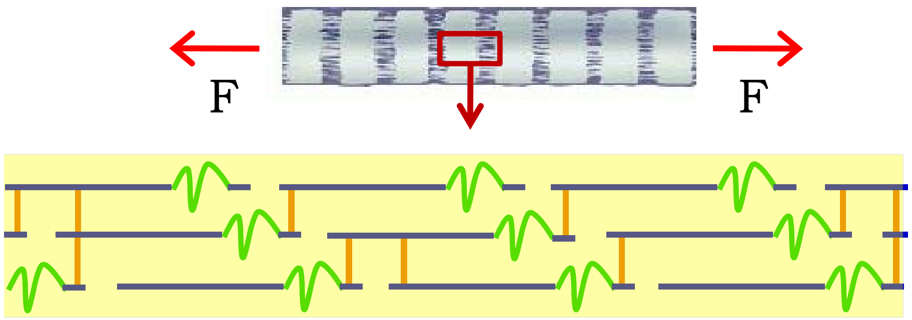
$\hat{\lambda}_p(z) =$ Occurrence parameter

$\hat{n}_{cl}(z) =$ Number of cross-links on fibril cross-section

A Model for Collagenous Fibrils

Loading

Homogeneous traction

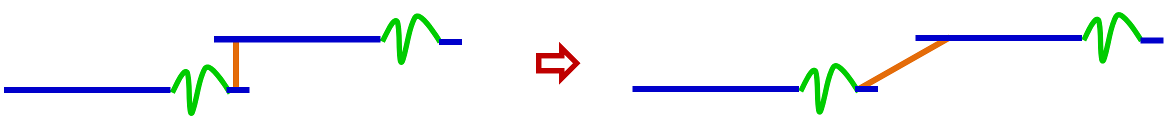


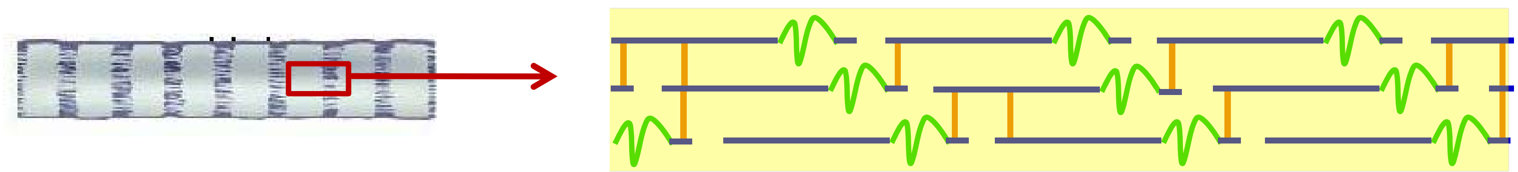
Kinematics

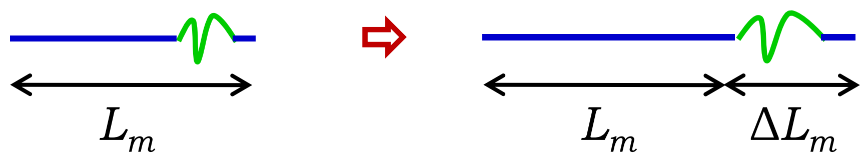
Two main deformation mechanisms:

-Molecular straightening:

-Cross-link straightening:







<u>Molecular state variables:</u> $\varepsilon_m = \dfrac{\Delta L_m}{L_m}$ $\beta_m \in [0,1]$ ⟵ Damage parameter:

$\beta_m = 0$ → cracked

$\beta_m = 1$ → sound

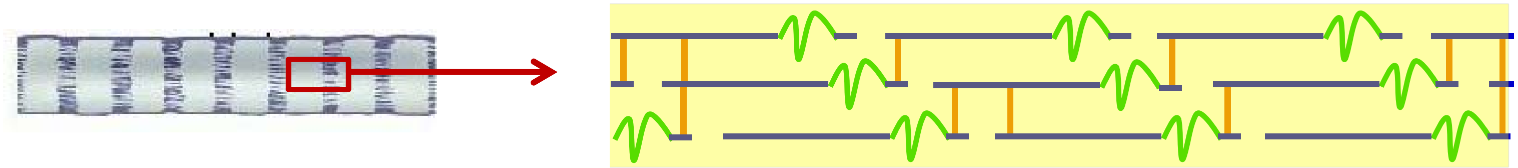
- Molecular free-energy density and dissipative pseudopotential density:

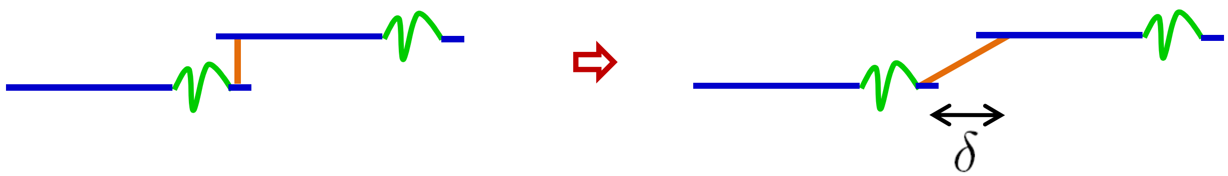
$$\Psi_m(\varepsilon_m, \beta_m)$$

Accounting for:
Entropic elasticity
Energetic elasticity

$$\Phi_m(\dot{\varepsilon}_m, \dot{\beta}_m)$$

Accounting for:
Brittle fracture





Cross-link state variables: δ $\beta_{cl} \in [0,1]$ ⟵ Damage parameter:
$\beta_{cl} = 0 \rightarrow$ cracked
$\beta_{cl} = 1 \rightarrow$ sound

- Cross-link free-energy and dissipative pseudopotential:

$$\mathcal{E}_{cl}(\delta, \beta_{cl})$$

Assuming:
Linear elastic behaviour

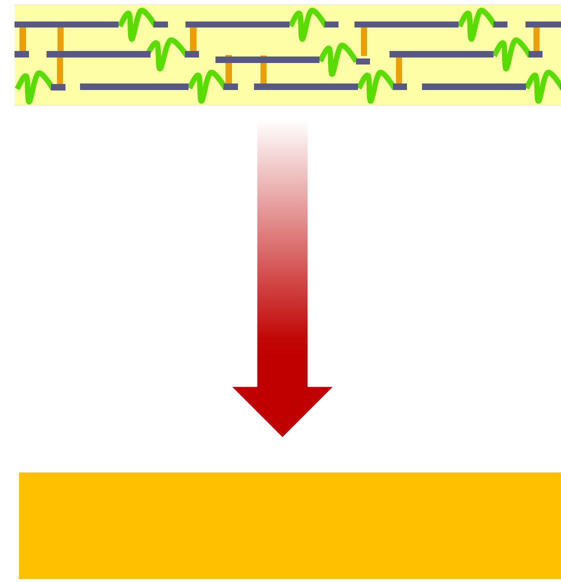
$$\mathcal{D}_{cl}(\dot{\delta}, \dot{\beta}_{cl})$$

Accounting for:
Ductile failure

Periodic geometry

$$\frac{L_m}{L_f} << 1$$

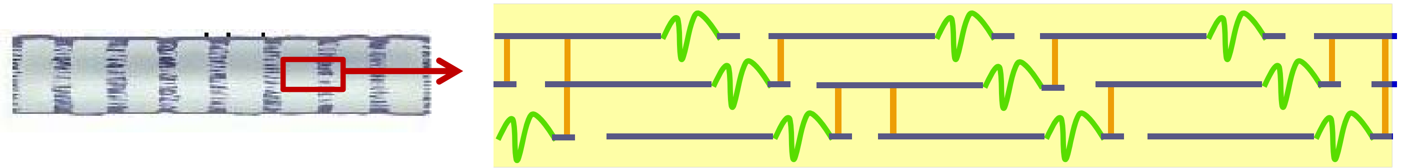
$$n_s \to +\infty$$



HOMOGENIZATION

Molecular and cross-links behaviour rule fibril's response

A Model for Collagenous Fibrils



$$N_m = n_s n_p$$

$$N_{cl} = \lambda N_m$$

Fibril's Free-Energy density:

$$\Psi_f = \frac{1}{\Omega_f}\int_{\cup\Omega_{m,i}} \Psi_{m,i}\, d\Omega + \frac{1}{\Omega_f}\sum_{i=1}^{N_{cl}} \mathcal{E}_{cl,i} \quad \xrightarrow{n_s \to +\infty} \quad \boxed{\Psi_f = \frac{\Psi_m}{\mu} + \frac{\lambda}{\mu\Omega_m}\mathcal{E}_{cl}}$$

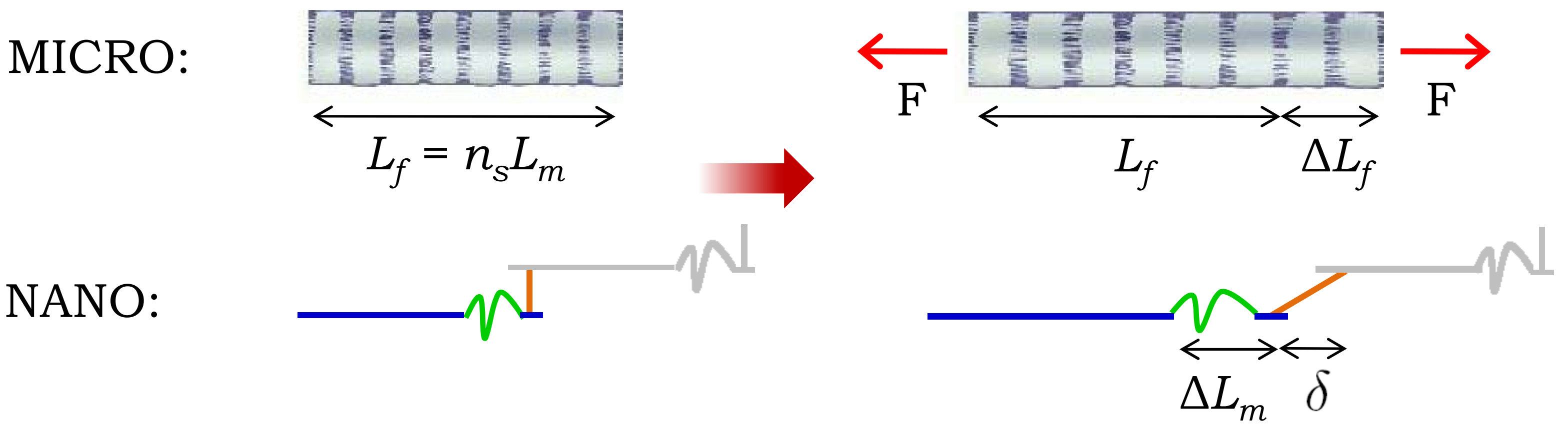
$( )_i = ( )_j = ( ) \quad (i \neq j)$

Fibril's dissipative pseudopotential density:

$$\Phi_f = \frac{1}{\Omega_f}\int_{\cup\Omega_{m,i}} \Phi_{m,i}\, d\Omega + \frac{1}{\Omega_f}\sum_{i=1}^{N_{cl}} \mathcal{D}_{cl,i} \quad \xrightarrow{n_s \to +\infty} \quad \boxed{\Phi_f = \frac{\Phi_m}{\mu} + \frac{\lambda}{\mu\Omega_m}\mathcal{D}_{cl}}$$

A MODEL FOR COLLAGENOUS FIBRILS

MICRO-NANO KINEMATIC COMPATIBILITY



Kinematic assumption:

$$\Delta L_f = n_s(\Delta L_m + \delta) \quad \rightarrow \quad \varepsilon_f = \frac{\Delta L_f}{L_f} = \frac{1}{\mu_s}\left(\varepsilon_m + \frac{\delta}{L_m}\right)$$

A Model for Collagenous Fibrils

Constitutive laws at nanoscale

Molecular stress:

$$\sigma_m = \frac{\partial \Psi_m}{\partial \varepsilon_m} + \frac{\partial \Phi_m}{\partial \dot{\varepsilon}_m}$$

Cross-link reactive force:

$$R = \frac{\partial \mathcal{E}_{cl}}{\partial \delta} + \frac{\partial \mathcal{D}_{cl}}{\partial \dot{\delta}}$$

Nanostress due to molecular damage:

$$b_m = \frac{\partial \Psi_m}{\partial \beta_m} + \frac{\partial \Phi_m}{\partial \dot{\beta}_m}$$

Nanoforce due to cross-link damage:

$$B_{cl} = \frac{\partial \mathcal{E}_{cl}}{\partial \beta_{cl}} + \frac{\partial \mathcal{D}_{cl}}{\partial \dot{\beta}_{cl}}$$

Constitutive laws at microscale

Fibril stress:

$$\sigma_f = \frac{\partial \Psi_f}{\partial \varepsilon_f} + \frac{\partial \Phi_f}{\partial \dot{\varepsilon}_f}$$

Cross-links total reactive force at fibrillar level:

$$R_f = \left(\frac{\partial \Psi_f}{\partial \delta} + \frac{\partial \Phi_f}{\partial \dot{\delta}} \right) \Omega_f$$

A Model for Collagenous Fibrils

Equilibrium at nanoscale

By the Principle of Virtual Powers: $\mathcal{P}_{int} = \mathcal{P}_{ext}$ $\qquad \dot{\varepsilon}_m = \dfrac{dv}{dz}$

$$\mathcal{P}_{int} = N_m \left(\int_{\Omega_m} \sigma_m \dot{\varepsilon}_m \, d\Omega + \int_{\Omega_m} b_m \dot{\beta}_m \, d\Omega \right) + \lambda N_m \left(R\dot{\delta} + B_{cl} \dot{\beta}_{cl} \right)$$

$$\mathcal{P}_{ext} = N_m \mathcal{F} \left[v(L_m) - v(0) \right] + \lambda N_m \mathcal{F}_{cl} \dot{\delta}$$

where σ_m, b_m, R, and B_{cl} are static quantities at nanoscale, dual to kinematic variables

Equilibrium equations: (Nanoscale)

$$\frac{d\sigma_m}{dz} = 0 \quad \text{for } z \in [0, L_m]$$

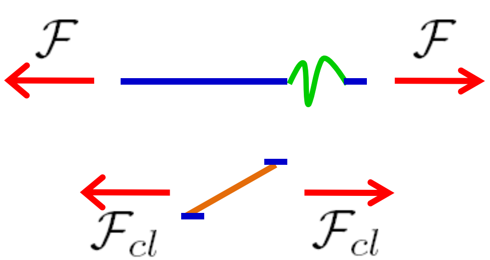
$$\mathcal{F} = \sigma_m A_m$$

$$\mathcal{F}_{cl} = R$$

$$b_m = 0$$

$$B_{cl} = 0$$

where:



Equilibrium at microscale

Nanoscale state variables:

$$(\varepsilon_m,\ \delta,\ \beta_m,\ \beta_{cl})$$

Microscale state variables:

$$(\varepsilon_f,\ \delta,\ \beta_m,\ \beta_{cl})$$

$$\varepsilon_f = \frac{1}{\mu_s}\left(\varepsilon_m + \frac{\delta}{L_m}\right)$$

By the Principle of Virtual Powers at the microscale:

$$\dot{\varepsilon}_f = \frac{dV}{dz}$$

$$\mathcal{P}_{int} = \int_{\Omega_f} \sigma_f \dot{\varepsilon}_f \, d\Omega + N_m \int_{\Omega_m} b_m \dot{\beta}_m \, d\Omega + R_f \dot{\delta} + \lambda N_m B_{cl} \dot{\beta}_{cl} \qquad \mathcal{P}_{ext} = F\left[V(L_f) - V(0)\right]$$

where σ_f and R_f are static quantities at microscale, dual to ε_f and δ.

Equilibrium equations: (Microscale)

$$\frac{d\sigma_f}{dz} = 0 \quad \text{for } z \in [0, L_f]$$

$$F = \sigma_f A_f$$

$$R_f = 0$$

$$b_m = 0$$

$$B_{cl} = 0$$

where:

A Model for Collagenous Fibrils

A bridge from nanoscale to microscale

By homogenization and compatibility:

$$\Psi_f(\varepsilon_m,\delta,\beta_m,\beta_{cl}) = \frac{\Psi_m(\varepsilon_m,\beta_m)}{\mu} + \frac{\lambda}{\mu\Omega_m}\mathcal{E}_{cl}(\delta,\beta_{cl}) \quad \Rightarrow \quad \Psi_f(\varepsilon_f,\delta,\beta_m,\beta_{cl})$$

$$\varepsilon_f = \frac{1}{\mu_s}\left(\varepsilon_m + \frac{\delta}{L_m}\right)$$

$$\Phi_f(\dot{\varepsilon}_m,\dot{\delta},\dot{\beta}_m,\dot{\beta}_{cl}) = \frac{\Phi_m(\dot{\varepsilon}_m,\dot{\beta}_m)}{\mu} + \frac{\lambda}{\mu\Omega_m}\mathcal{D}_{cl}(\dot{\delta},\dot{\beta}_{cl}) \quad \Rightarrow \quad \Phi_f(\dot{\varepsilon}_f,\dot{\delta},\dot{\beta}_m,\dot{\beta}_{cl})$$

$$\Rightarrow \quad \boxed{\sigma_m = \sigma_f\,\mu_p} \qquad \boxed{R_f = \left(\frac{\partial\Psi_f}{\partial\delta} + \frac{\partial\Phi_f}{\partial\dot{\delta}}\right)\Omega_f = \lambda N_m\left(R - \frac{\mathcal{F}}{\lambda}\right)}$$

By equilibrium:

$$\mathcal{F} = \sigma_m A_m$$
$$\mathcal{F}_{cl} = R$$
$$F = \sigma_f A_f$$
$$R_f = 0$$

$$\Rightarrow \quad \mathcal{F}_{cl} = \frac{\mathcal{F}}{\lambda} \quad \rightarrow \quad \sigma_m = \frac{\lambda}{A_m}R \quad \rightarrow \quad \frac{\partial\Psi_m}{\partial\varepsilon_m} + \frac{\partial\Phi_m}{\partial\dot{\varepsilon}_m} = \frac{\lambda}{A_m}\frac{\partial\mathcal{E}_{cl}}{\partial\delta} + \frac{\partial\mathcal{D}_{cl}}{\partial\dot{\delta}}$$

OUTLINE

⟹ Mechanics of soft tissues: macroscale → nanoscale

⟹ **A multiscale elasto-damaging model for collagenous fibrils**:

- **Nanoscale: Molecular model**
- Nanoscale: Cross-links model
- Microscale: Fibril model

⟹ Conclusions and Perspective: Back to the macroscale

Free-energy density:

$$\mathrm{I}(x) = \begin{cases} 0 & \text{if } x \in [0,1] \\ +\infty & \text{elsewhere} \end{cases}$$

$$\Psi_m(\varepsilon_m, \beta_m) = \beta_m \Psi_m^{el}(\varepsilon_m) + (1-\beta_m) w_m + \mathrm{I}(\beta_m)$$

Threshold of damage activation

Dissipative pseudopotential density:

$$\Phi_m(\dot{\varepsilon}_m, \dot{\beta}_m) = c_m \frac{\dot{\beta}_m^2}{2} + \mathrm{I}_-(\dot{\beta}_m)$$

Irreversibility condition for damage evolution

It will give linear dependence for the evolution of damage

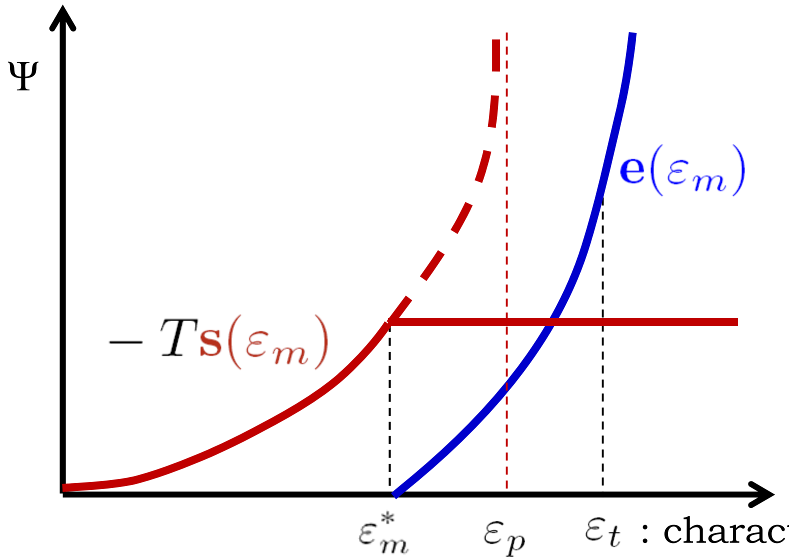
$$\mathrm{I}_-(x) = \begin{cases} 0 & \text{if } x \in \mathbb{R}^- \\ +\infty & \text{elsewhere} \end{cases}$$

Free-energy density:

$$\mathrm{I}(x) = \begin{cases} 0 & \text{if } x \in [0,1] \\ +\infty & \text{elsewhere} \end{cases}$$

$$\Psi_m(\varepsilon_m, \beta_m) = \beta_m \Psi_m^{el}(\varepsilon_m) + (1-\beta_m) w_m + \mathrm{I}(\beta_m)$$

$$\Psi_m^{el}(\varepsilon_m) = \mathbf{e}(\varepsilon_m) - T\mathbf{s}(\varepsilon_m)$$



ε_t : characteristic point of energetic elasticity

Two parameters are linked with physical nano-scale mechanisms :

$$(\varepsilon_m^*, \varepsilon_t)$$

Note that: $\varepsilon_m^* < \varepsilon_p$

$$\Psi_m^{el}(\varepsilon_m) = \mathbf{e}(\varepsilon_m) - T\mathbf{s}(\varepsilon_m) \ : \ \sigma_m(\varepsilon_m^*) = \left.\frac{\partial s}{\partial \varepsilon_m}\right|_{\varepsilon_m^*} = \left.\frac{\partial e}{\partial \varepsilon_m}\right|_{\varepsilon_m^*}$$

Elastic modulus in entropic elasticity:

$$s(\varepsilon_m) \ : \ E^s(\varepsilon_m) = \frac{\partial^2 s}{\partial \varepsilon_m^2} = r_a \left\{ \frac{r_\ell}{2\left[1 - r_\ell(\varepsilon_m + 1)\right]^3} + r_\ell \right\}$$

→ Recovery of the classical formulation for entropic elasticity (Worm-Like Chain model)

$$r_a = \frac{k_B T}{A_m L_p} \qquad r_\ell = \frac{L_m}{L_c}$$

Elastic modulus in energetic elasticity

$$e(\varepsilon_m) \ : \ E^e(\varepsilon_m) = \frac{\partial^2 e}{\partial \varepsilon_m^2} = \frac{\widehat{E}}{1 + e^{-m(\varepsilon_m - \varepsilon_t)}}$$

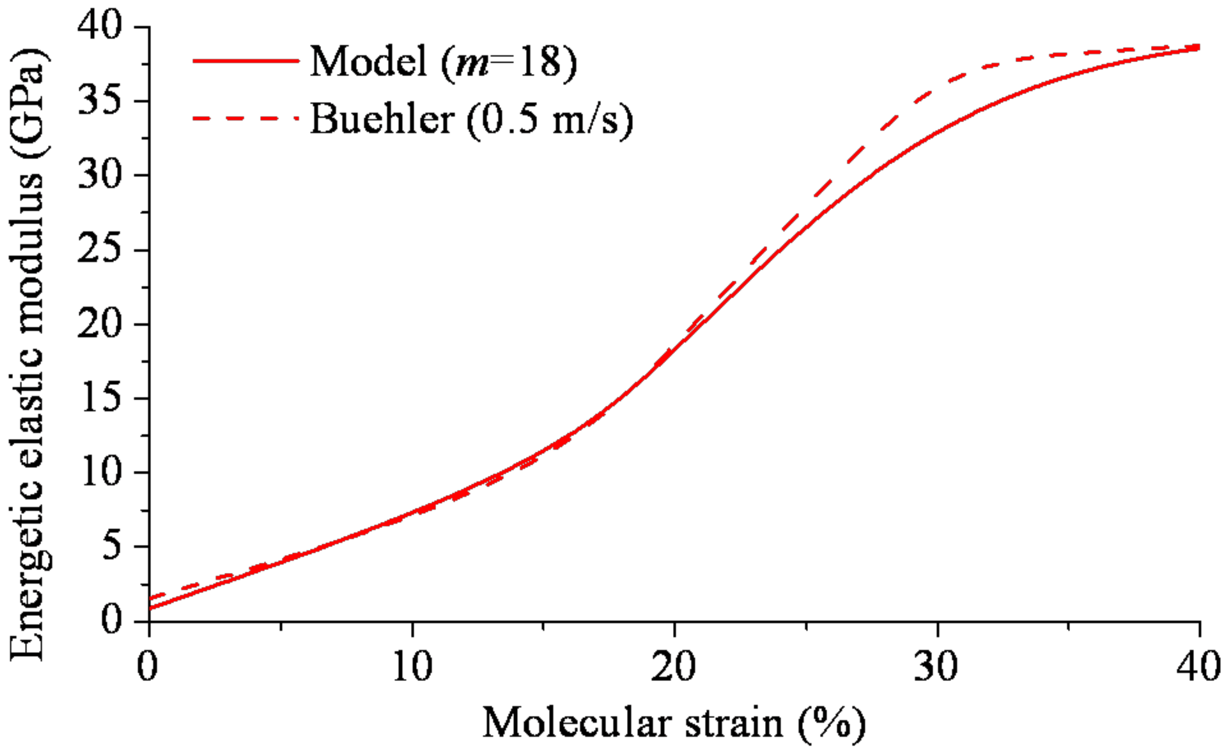
→ Compliant to results in Bueheler (2009) for non-linear energetic elasticity

Requirements:
$$\begin{cases} E^s(\varepsilon_m^*) = E^e(\varepsilon_m^*) \\ \left.\frac{\partial E^s}{\partial \varepsilon_m}\right|_{\varepsilon_m^*} = \left.\frac{\partial E^e}{\partial \varepsilon_m}\right|_{\varepsilon_m^*} \end{cases}$$
→ Uniqueness of $(\varepsilon_m^*, \varepsilon_t)$

MODEL VALIDATION:
ENERGETIC ELASTICITY

$$E^e(\varepsilon_m) = \frac{\partial^2 e}{\partial \varepsilon_m^2} = \frac{\widehat{E}}{1 + e^{-m(\varepsilon_m - \varepsilon_t)}}$$

Benchmarks on an isolated straight molecule (i.e, $\varepsilon_m \equiv$ molecular material strain)

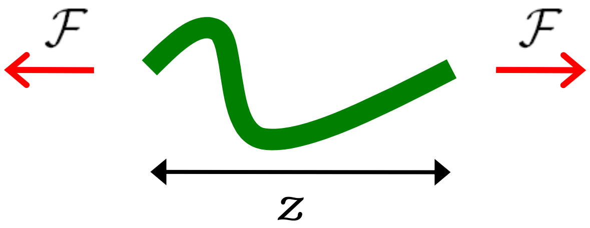


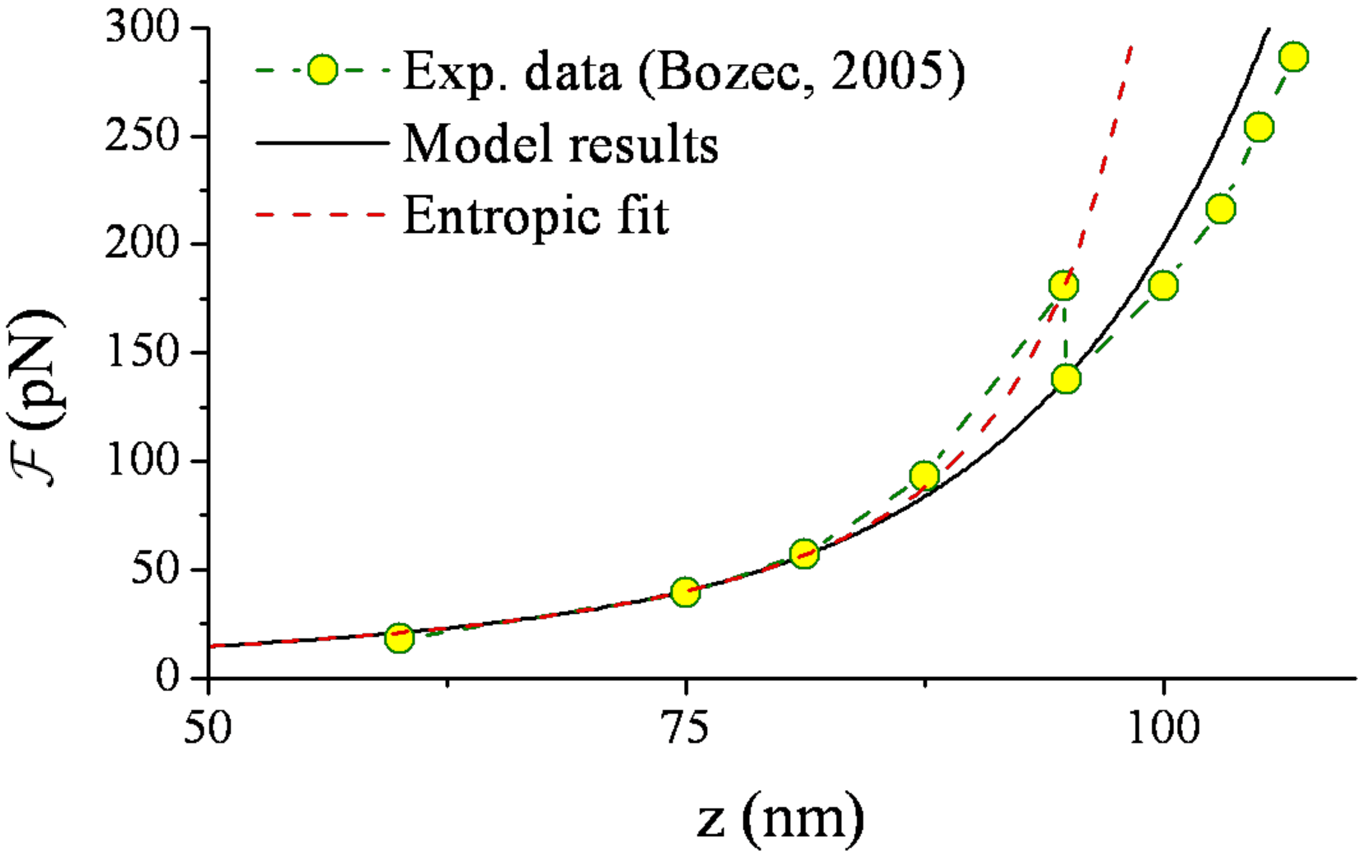
$\widehat{E}$: upper bound of collagen elastic modulus (40 GPa)

m: parameter dependent on deformation rate

ε_t : characteristic point of the given evolution law

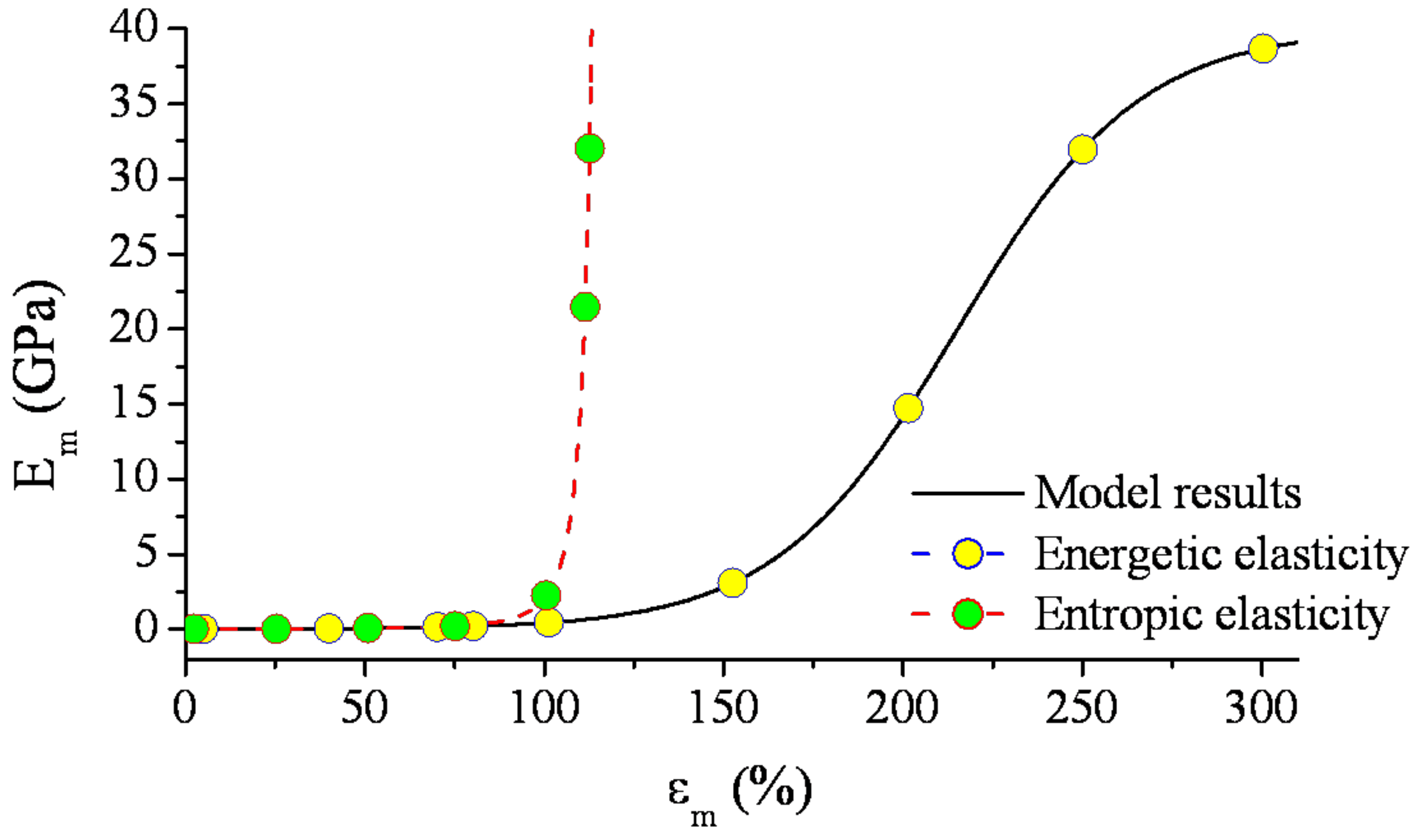
MODEL VALIDATION:
ENTROPIC + ENERGETIC MODEL





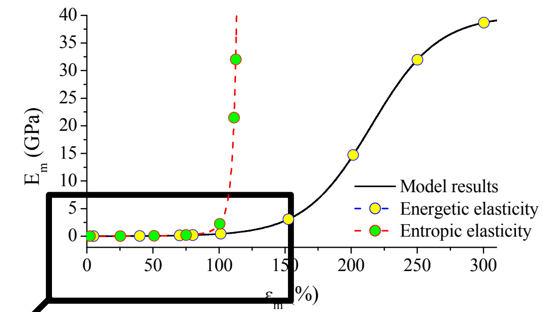
MODEL VALIDATION:
ENTROPIC TO ENERGETIC TRANSITION

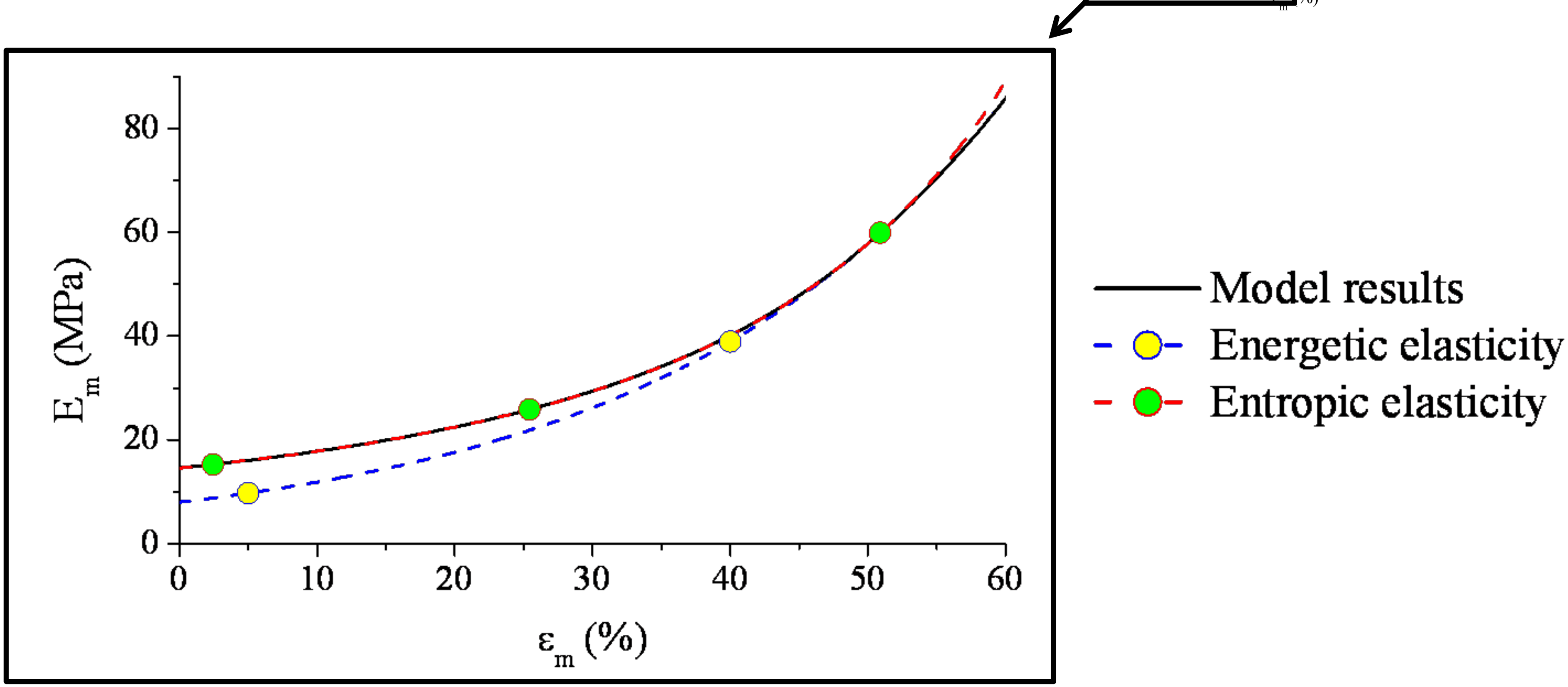
Equivalent elastic modulus of a collagen molecule:



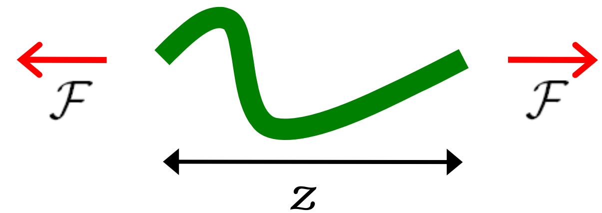
MODEL VALIDATION:
ENTROPIC TO ENERGETIC TRANSITION

Equivalent elastic modulus of a collagen molecule:

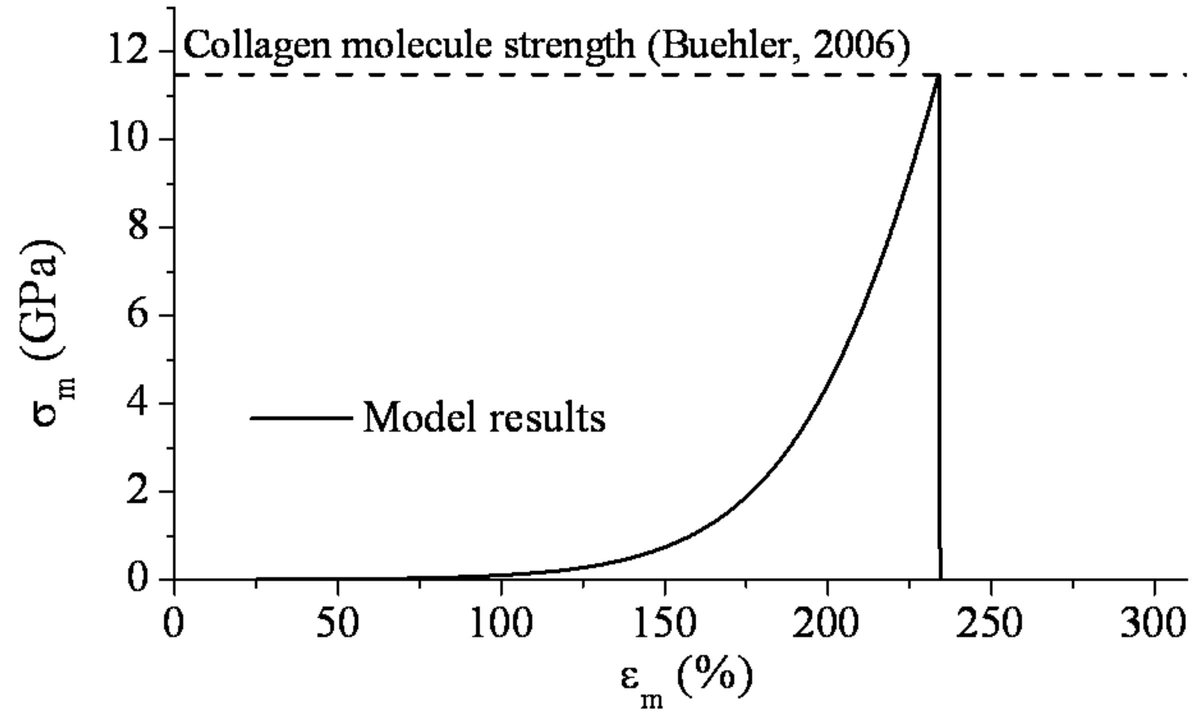




MODEL VALIDATION:
MOLECULAR BREAKAGE



Collagen strength and brittle-like mechanism are accurately reproduced ($w_m \approx 1{,}8$ J, $c_m = 10^{-3}$)



OUTLINE

⇒ Mechanics of soft tissues: macroscale → nanoscale

⇒ **A multiscale elasto-damaging model for collagenous fibrils**:

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⇒ Conclusions and Perspective: Back to the macroscale

Free-energy:

$$\mathrm{I}(x) = \begin{cases} 0 & \text{if } x \in [0,1] \\ +\infty & \text{elsewhere} \end{cases}$$

$$\mathcal{E}_{cl} = \beta_{cl} \frac{\rho k}{2} \delta^2 + (1 - \beta_{cl}) w_{cl} + \mathrm{I}(\beta_{cl})$$

w_{cl}: Threshold of damage activation

ρ : parameter expressing covalent bonds density within a cross-link
k : stiffness of a covalent bond

Dissipative pseudopotential:

$$\mathrm{I}_-(x) = \begin{cases} 0 & \text{if } x \in \mathbb{R}^- \\ +\infty & \text{elsewhere} \end{cases}$$

$$\mathcal{D}_{cl} = c_{cl} \frac{\dot{\beta}_{cl}^2}{2} + (1 - \beta_{cl}) \rho \bar{f} \| \dot{\delta} \| + \mathrm{I}_-(\dot{\beta}_{cl})$$

$\mathrm{I}_-(\dot{\beta}_{cl})$: Irreversibility condition

$\frac{\dot{\beta}_{cl}^2}{2}$: It will give linear dependence for the evolution of damage quantity

$(1 - \beta_{cl}) \rho \bar{f} \| \dot{\delta} \|$: Dissipative yield term
$\bar{f}$: cross-link yield force

OUTLINE

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⇒ Conclusions and Perspective: Back to the macroscale

Equilibrium Equations:

$$\sigma_m = \frac{\lambda}{A_m} R \quad \Rightarrow \quad \beta_m \frac{\partial \Psi_m^{el}}{\partial \varepsilon_m} = \frac{\lambda}{A_m} \left[\beta_{cl} \rho k \delta + (1 - \beta_{cl}) \rho \bar{f} G(\dot{\delta}) \right]$$

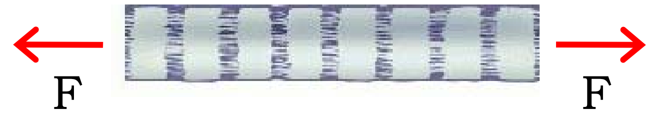
$$G(\dot{\delta}) = \begin{cases} 1 & \text{if } \dot{\delta} \neq 0 \\ p \, : \, |p| \leq 1 & \text{if } \dot{\delta} = 0 \end{cases}$$

Damage evolution laws:

$$b_m = 0 \quad \Rightarrow \quad c_m \dot{\beta}_m + \partial I(\beta_m) + \partial I_-(\dot{\beta}_m) \ni \left(w_m - \Psi_m^{el}(\varepsilon_m, T) \right)$$

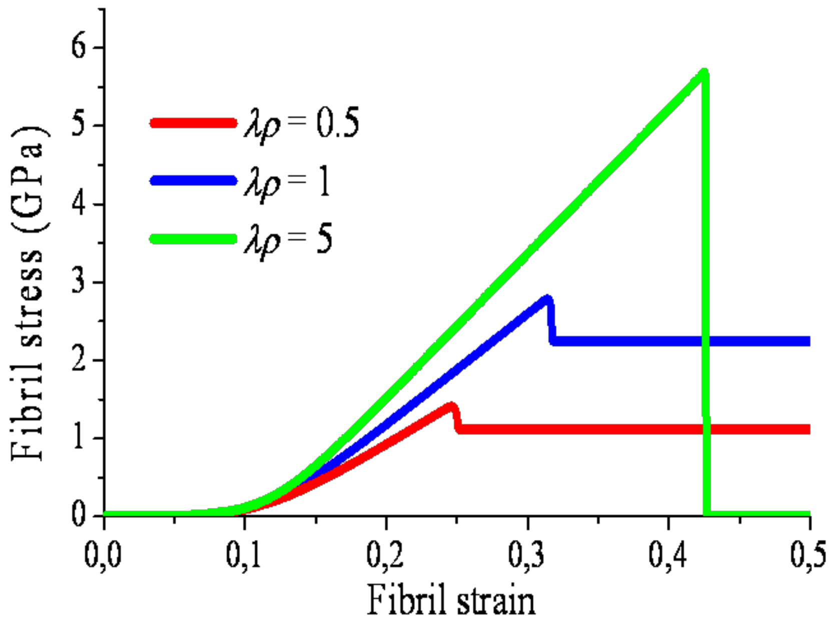
$$B_{cl} = 0 \quad \Rightarrow \quad c_{cl} \dot{\beta}_{cl} + \partial I(\beta_{cl}) + \partial I_-(\dot{\beta}_{cl}) \ni \left(w_{cl} - \frac{\rho k}{2} \delta^2 \right)$$

MODEL VALIDATION:

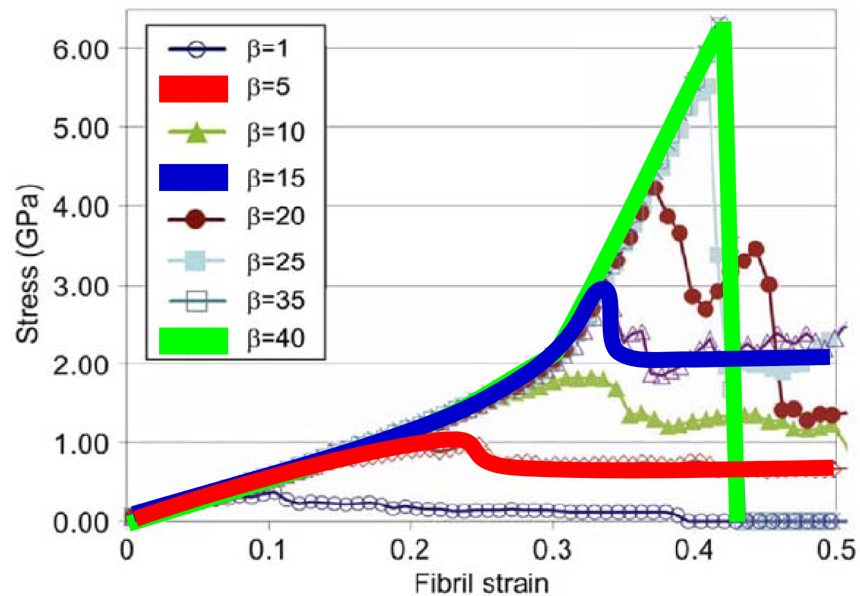


$\lambda\rho = 1 \leftrightarrow \beta = 15$ ($\rightarrow$ 1 covalent cross-link/molecule)

Model results:



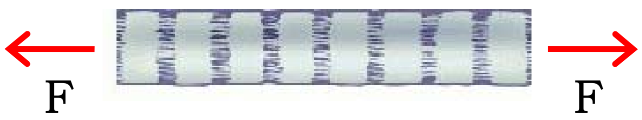
Dynamical molecular simulations:
(Buehler, 2008)



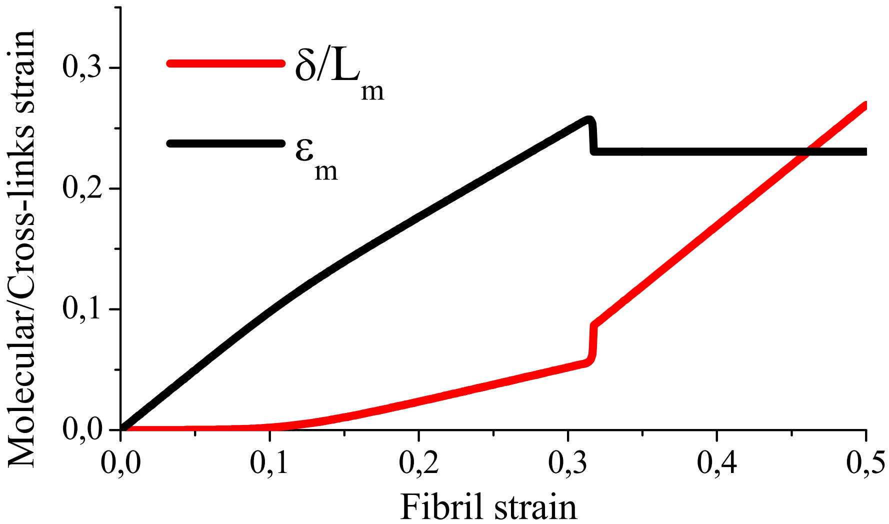
$\lambda\rho \approx$ cross-links density

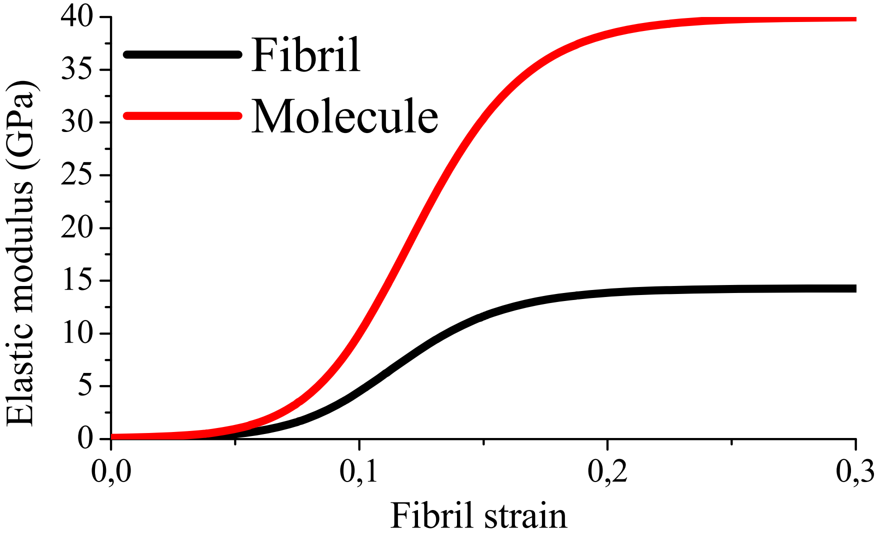
MODEL RESULTS:

$\lambda\rho=1$



Nano-scale deformation mechanisms
are effectively taken into account at the micro-scale





Model takes into account the hierarchical and organized structure of collagen fibrils

OUTLINE

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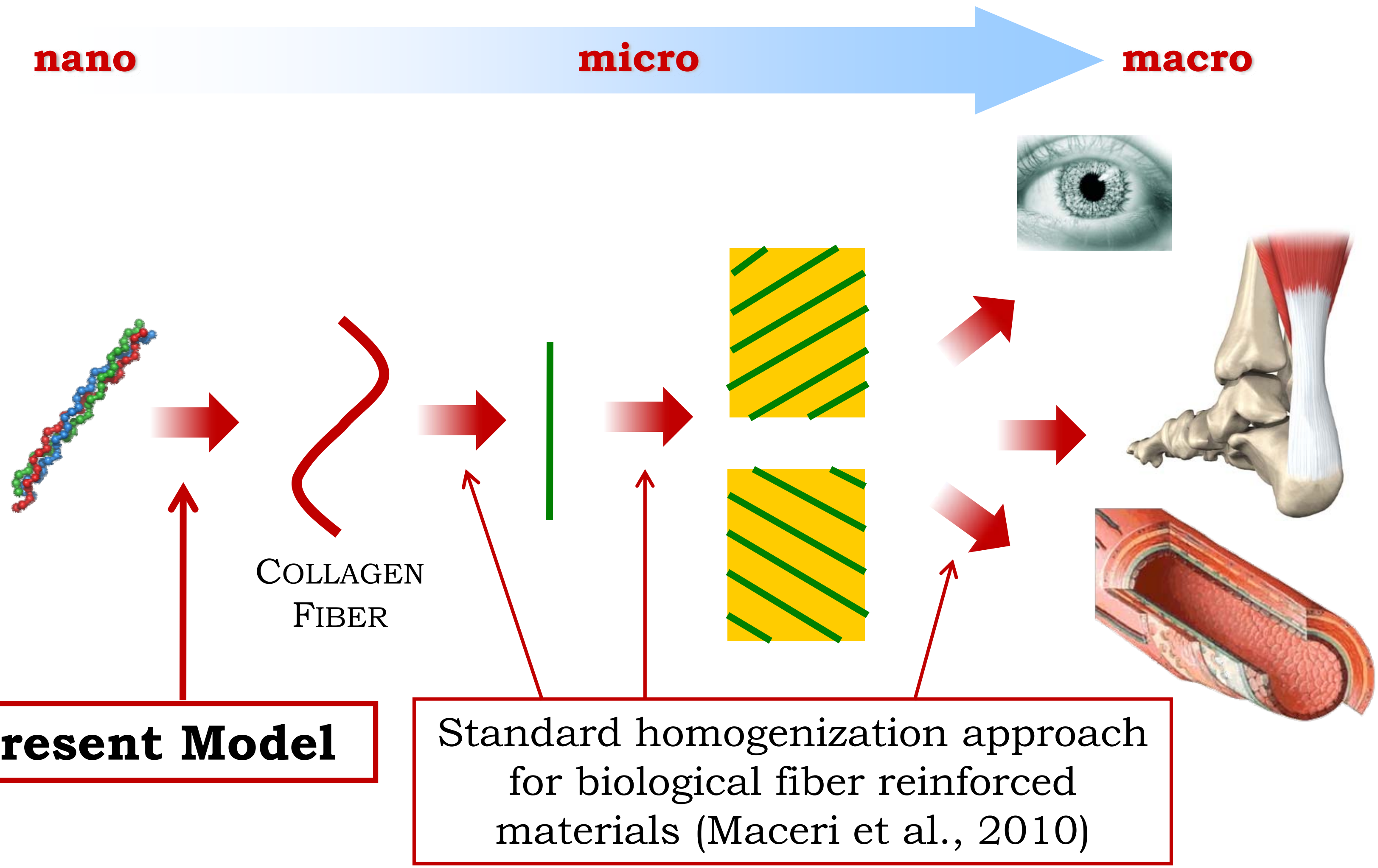
⇒ **Conclusions and Perspective: Back to the macroscale**

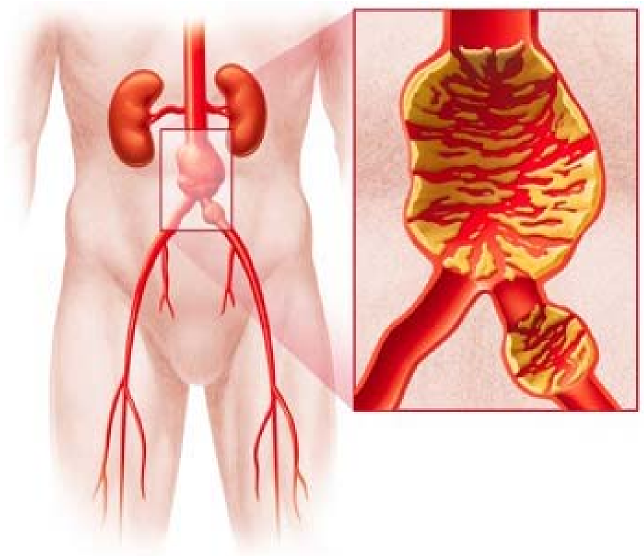
CONCLUSIONS AND PERSPECTIVE

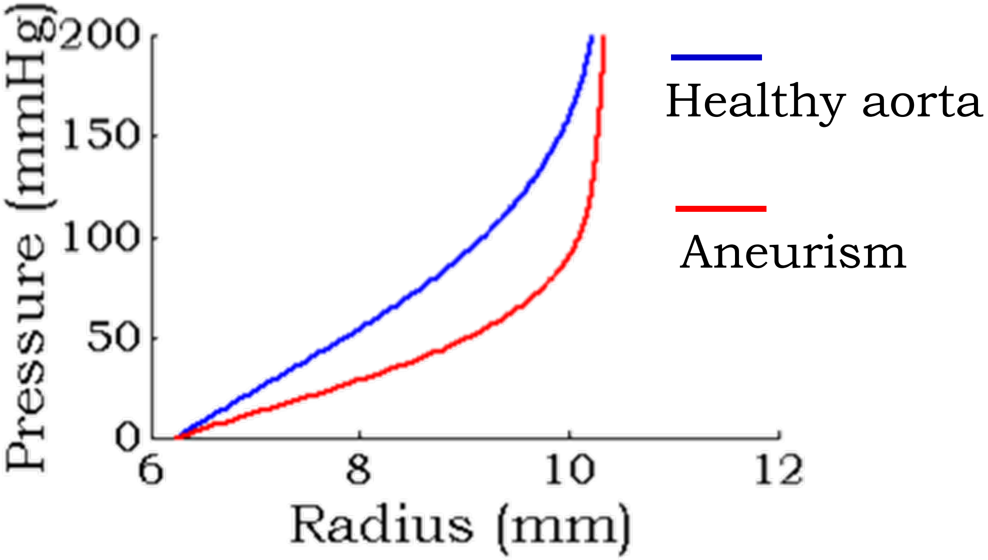
BACK TO THE MACROSCALE



BACK TO THE MACROSCALE

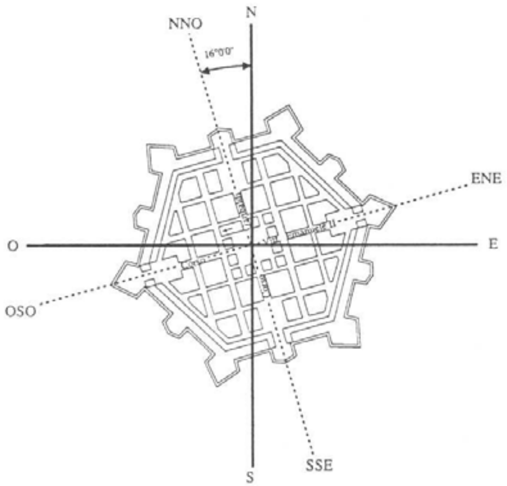
Lamellar unit degradation (-50%) is a key factor in the development of aneurismal dilatation (Zatina,1984 – Wilson,1999)





F. Maceri, M. Marino, G. Vairo (2010) *A unified multiscale mechanical model for soft collagenous tissues with regular fiber arrangement*, J. Biomechanics **43**:355-363

Thank You



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