Experiments and nonlocal continuum modeling of the size-dependent fracture in elastomers[1,2]

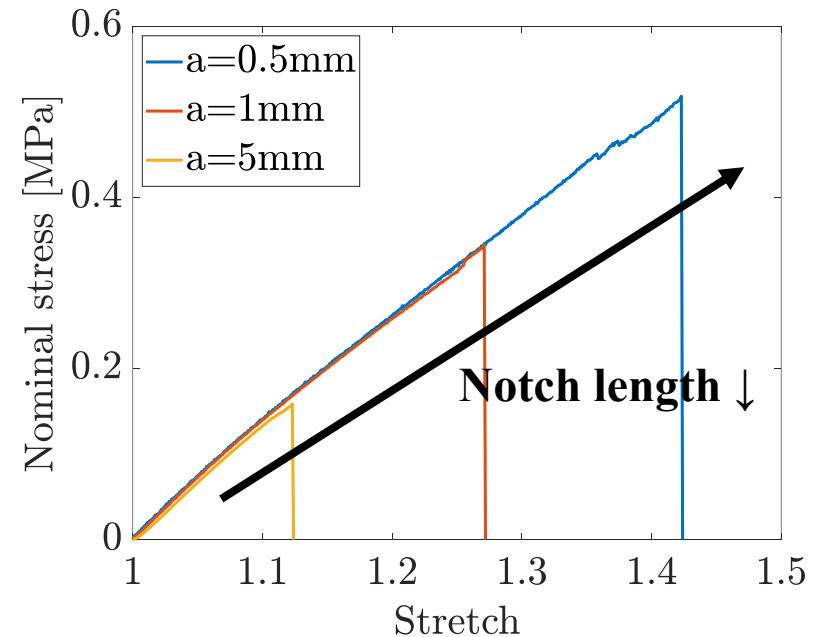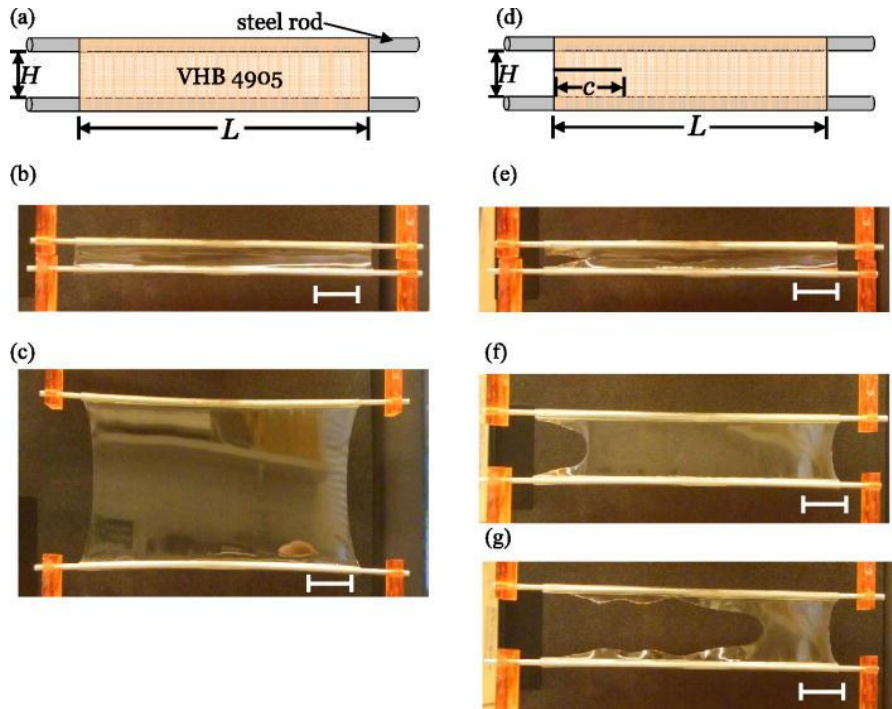Jeongun Lee, Jaehee Lee and Hansohl Cho*

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Mechanics & Extremes
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Fracture in elastomers

- Extreme, nonlinear deformation → nonlinear fracture

- Influenced by the size of flaws; **the size-dependent fracture**[1,3]

 - Rupture stretch increases as the specimen size decreases

a) The presence of flaws impacts the fracture behavior[4]

b) Size-dependent fracture in polydimethylsiloxane (PDMS) specimens

Fracture in elastomers

- Occurs when …

  - Macroscopically, **G reaches Γ**

    - Griffith theory[5,6]

    - G: Energy release rate

    - Γ: Fracture energy

$$G = -\frac{dU(\mathrm{P}, \Delta)}{dA}$$

- Microscopically, $\boldsymbol{\varepsilon_R}$ **reaches** $\boldsymbol{\varepsilon_R^f}$

  - Lake-Thomas theory[7-9]

  - ε_R: Internal energy

  - ε_R^f: critical internal energy;
        bond dissociation energy

- These approaches are compatible (Lake and Thomas [7])
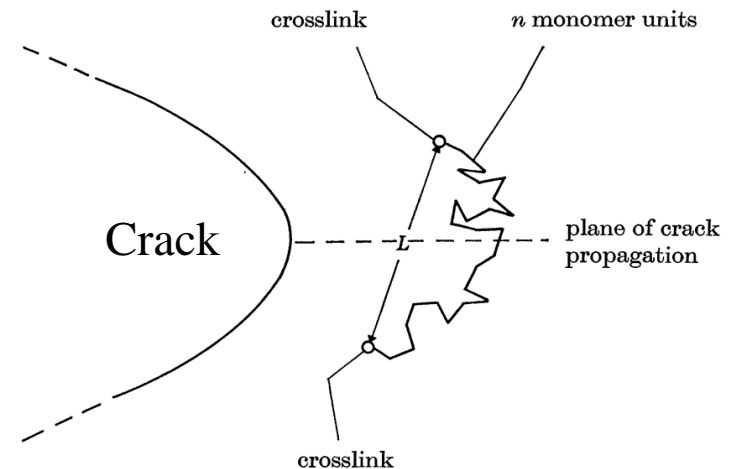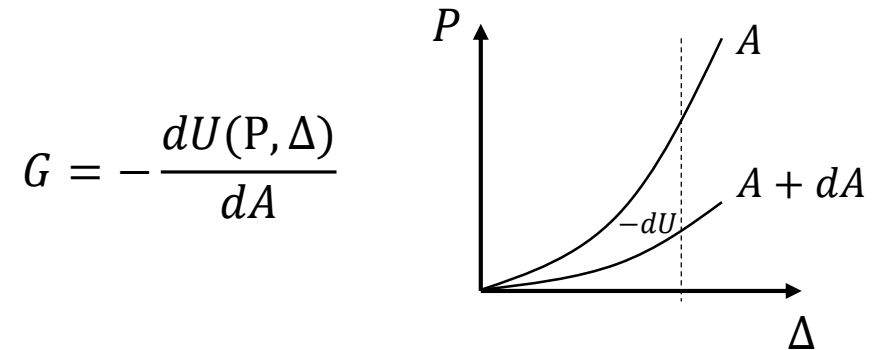
Objectives

- Predicting the **size-dependent fracture** in elastomers[1]

  - Experiments and numerical simulations[2] were carried out

- **Internal energy-driven** fracture criterion; inspired by the Lake-Thomas model[7-9]

- Using the **phase-field model** rooted in the gradient-damage theory[2,9-13]

  - Mesh-insensitive crack propagation process

  - The internal energy-driven fracture criterion

  - Thermodynamics of the damage and fracture

Size-dependent fracture & Fracture process zone

- Fracture process zone
  - Where the polymer chains rupture = Where the dissipation mainly occurs

- Stress at point (B) is larger than those at (A) and (A')
  - $\sigma_A = \sigma_{A'} < \sigma_B$

- → Free energy at point (B) is larger than those at (A) and (A')
  - $\psi_A = \psi_{A'} < \psi_B$

- → ψ_B **reaches the critical energy earlier than** ψ_A

- → **The larger specimen ruptures earlier**

The size of fracture process zone[1,3,14,15]:

$$l = \frac{\Gamma}{W^*} = \frac{Fracture\ energy}{Critical\ deformation\ energy}$$

(B) (A')

(A)
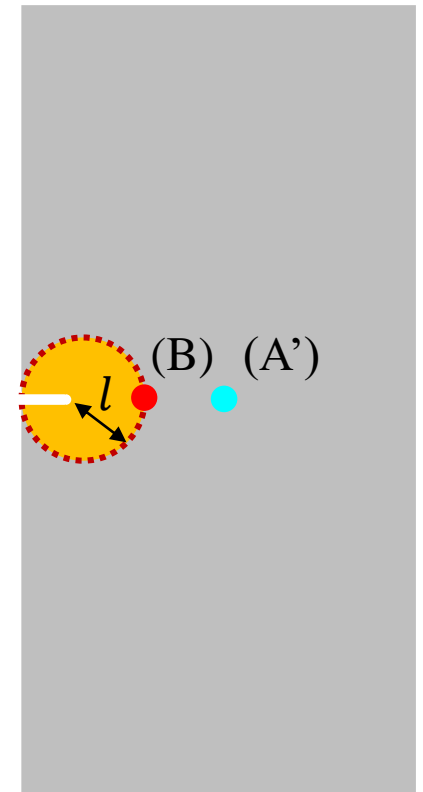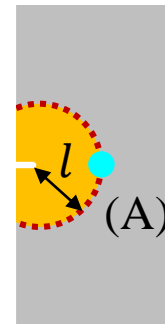
Nonlocal continuum modeling

- 1. The damage $d \in [0,1]$
  - d=0: intact
  - d=1: fully damaged

- **Internal energy-driven** fracture criterion
  - Inspired by the Lake-Thomas model[5]
  - Fracture = **Scission of polymer chains**

- Governing equations[9]
  - Macroforce balance   Div $\mathbf{T}_R = 0$
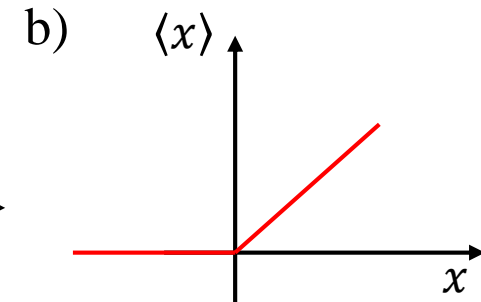 - Microforce balance $\zeta \dot{d} = 2(1-d)\mathcal{H}_R - \hat{\varepsilon}_R^f(d - l'^2 \Delta d)$
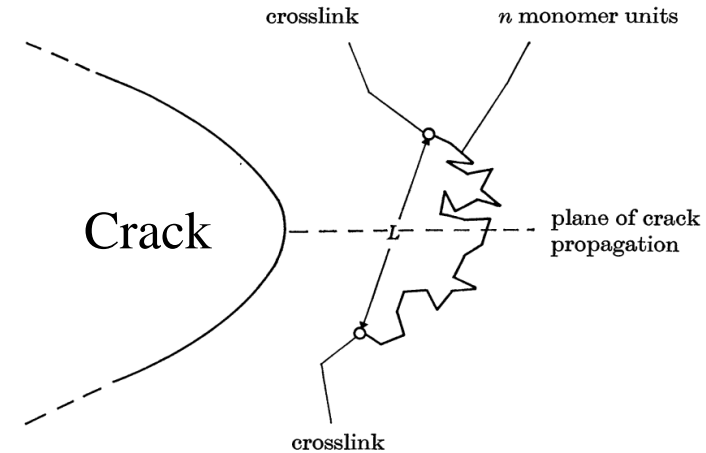
History function;
the fracture criterion

$$\mathcal{H}_R = \left\langle \varepsilon_R^0 - \varepsilon_R^f/2 \right\rangle, \quad \text{where } \langle x \rangle = \begin{cases} x & if \ x > 0 \\ 0 & if \ x \leq 0 \end{cases}$$

Internal energy

a)[7]

crosslink n monomer units

Crack

plane of crack propagation
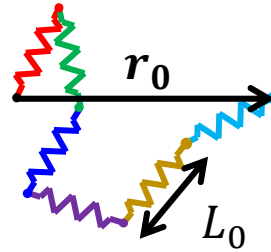
crosslink

b) $\langle x \rangle$

x

Nonlocal continuum modeling
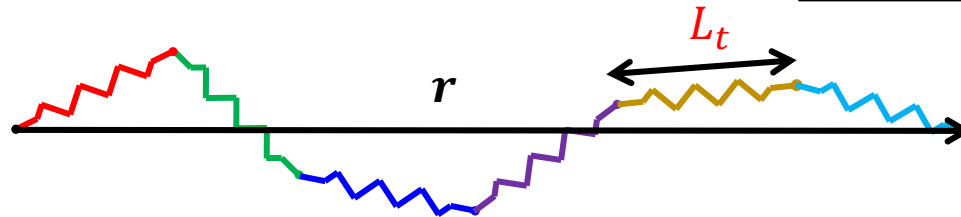
- **Internal energy** should be considered → **Bond stretch**[8,9]

  - Deformation = Chain configuration change + stretching of molecular bonds

- $\psi_R = (1-d)^2 \left[\frac{1}{2} NnE_b(\lambda_b - 1)^2 + \frac{1}{2}K(J-1)^2 \right] + Nk_b\theta n \left[\frac{\bar{\lambda}\lambda_b^{-1}}{\sqrt{n}}\beta + \ln\left(\frac{\beta}{\sinh\beta}\right) \right] + \frac{1}{2}\varepsilon_R^f l^2 |\nabla d|^2$

$(1-d)^2\varepsilon_R^0$; **Damage acts on the internal energy only** $\quad -\theta\eta_R$; Entropic energy $\quad$ Nonlocal energy[9]

a) Reference configuration

r_0

L_0

a) Deformed configuration

L_t

r

$$\bar{\lambda} = \frac{|\boldsymbol{r}|}{|\boldsymbol{r_0}|}$$

$$\lambda_b = \frac{L_t}{L_0}$$

$$\mathcal{L}(x) = \coth x - \frac{1}{x}$$

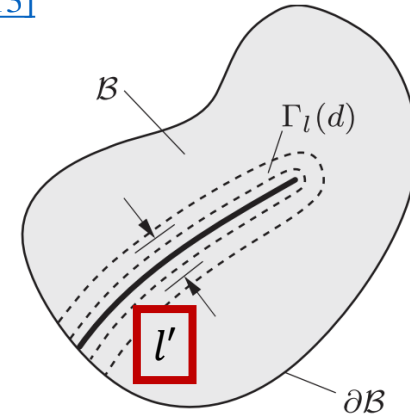$$\beta = \mathcal{L}^{-1}\left(\frac{\bar{\lambda}\lambda_b^{-1}}{\sqrt{n}}\right)$$

Nonlocal continuum modeling

- 2. Phase-field model rooted in the gradient-damage theory[9-13]

  - "Diffusive damage zone"

a)[13]

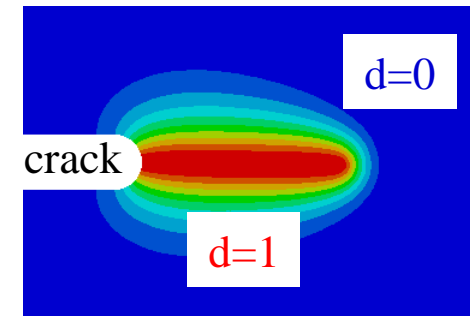**Intrinsic length scale l'**

- Microforce balance $\zeta\dot{d} = 2(1-d)\mathcal{H}_R - \hat{\varepsilon}_R^f(d - \boxed{l'^2\Delta d})$

  History function;
  the fracture criterion

- The **intrinsic length scale l'** → the size of diffusive damage zone

  - A numerical parameter; ambiguous physical meaning

b)

Crack propagation;
at reference configuration

Nonlocal continuum modeling

- Assumption[1]: Diffusive damage zone = Fracture process zone

  - Regions of the damage evolution and the dissipation
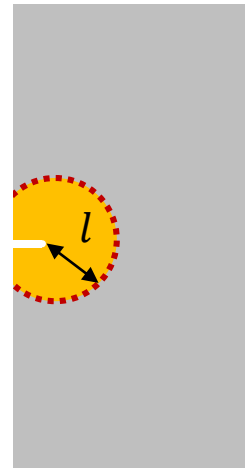
- The size of fracture process zone

$$= \frac{\Gamma}{W^*} = \frac{Fracture\ energy}{Critical\ deformation\ energy}$$ → **Intrinsic length scale**

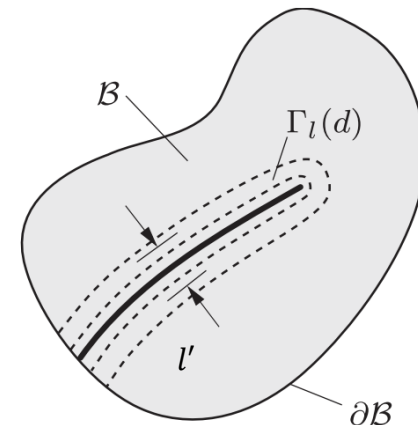→ Identify the intrinsic length scale l **from experiments**

→ Apply to the phase field model

→ Predict the **size-dependent fracture** by numerical simulations[1]
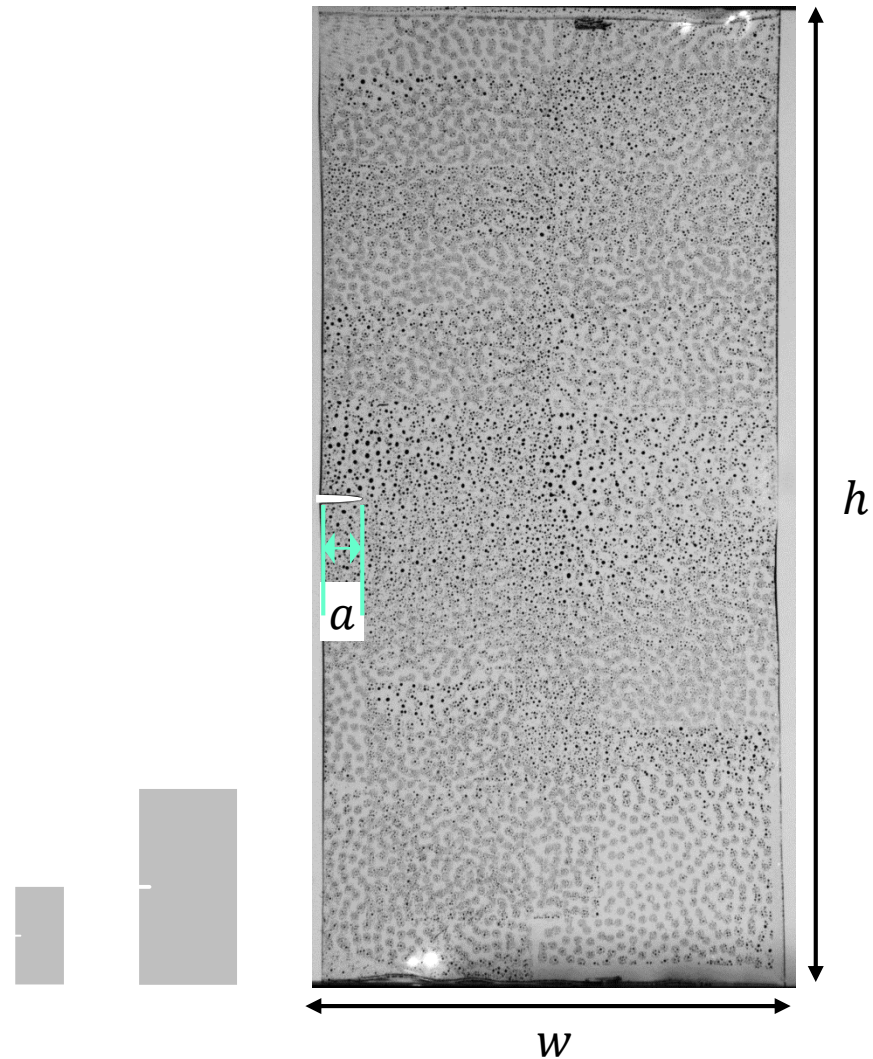
a) Fracture process zone

b)[13] Diffusive damage zone

Experimental procedures[1]

- Geometries

  - a = {0.5, 1, 5} mm

  - w = 10a, h = 20a, specimen thickness: 0.5mm

    → w = {5, 10, 50} mm

    → h = {10, 20, 100} mm

- Materials

  - PDMS

  - TangoPlus (3D-printed elastomer)

- Strain rate 0.01 s^{-1}, temperature ~21℃

- Digital image correlation (DIC) analysis

  → Strain fields from experiments

The intrinsic length scale l

- $l = \frac{\Gamma}{W^*}$ → **Experimentally identified intrinsic length scale**[1]

- Γ: Fracture energy
  - from notched specimens

- W^*: Critical deformation energy
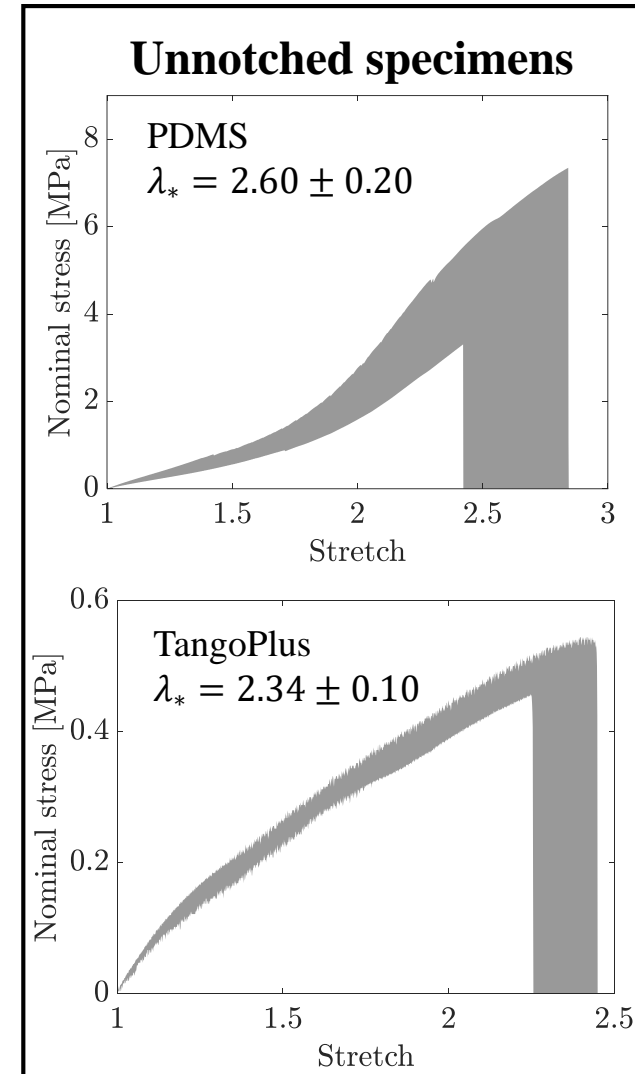 - from unnotched specimens

PDMS

$\Gamma \approx 0.25\text{mJ/mm}^2, W^* \approx 2.7\text{mJ/mm}^3$
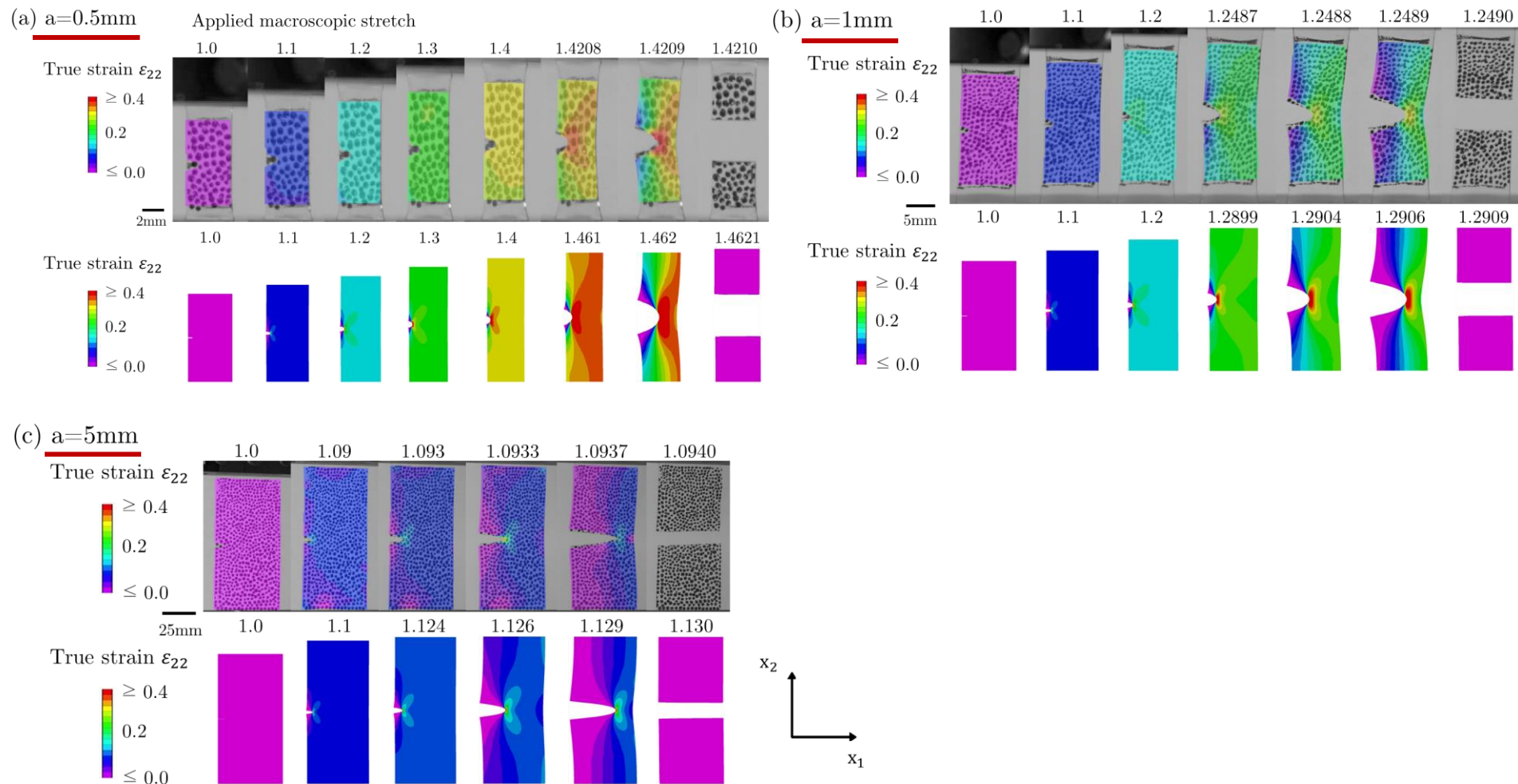
→ $l \approx 0.08mm$

TangoPlus

$\Gamma = 0.5\text{mJ/mm}^2, W^* \approx 0.45\text{mJ/mm}^3$

→ $l \approx 1mm$

Unnotched specimens

PDMS
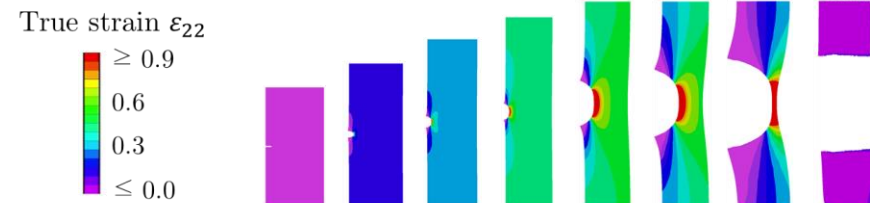$\lambda_* = 2.60 \pm 0.20$
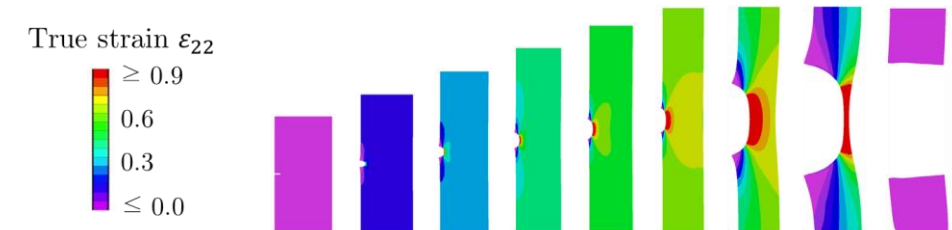
TangoPlus
$\lambda_* = 2.34 \pm 0.10$

Results: Experiment vs. Numerical simulation[1]

- Strain fields in **PDMS** specimens ($l = 0.08mm$)

  - Larger specimen ruptures earlier

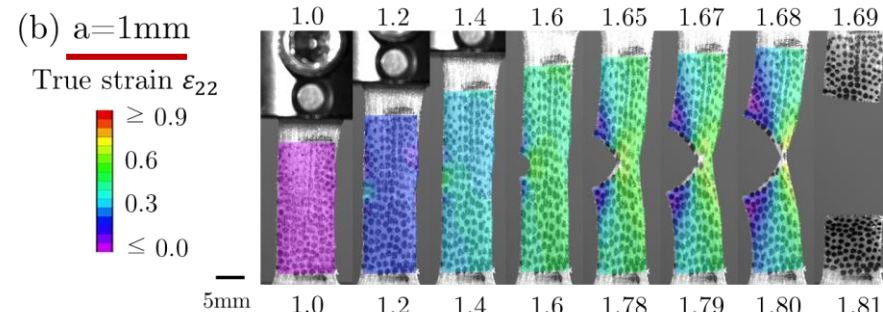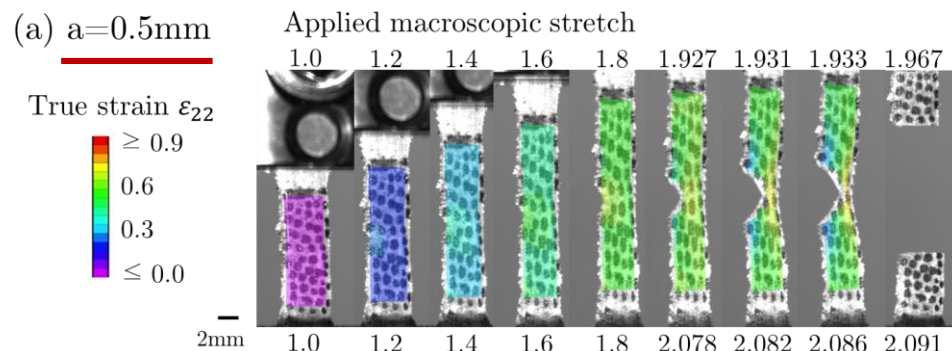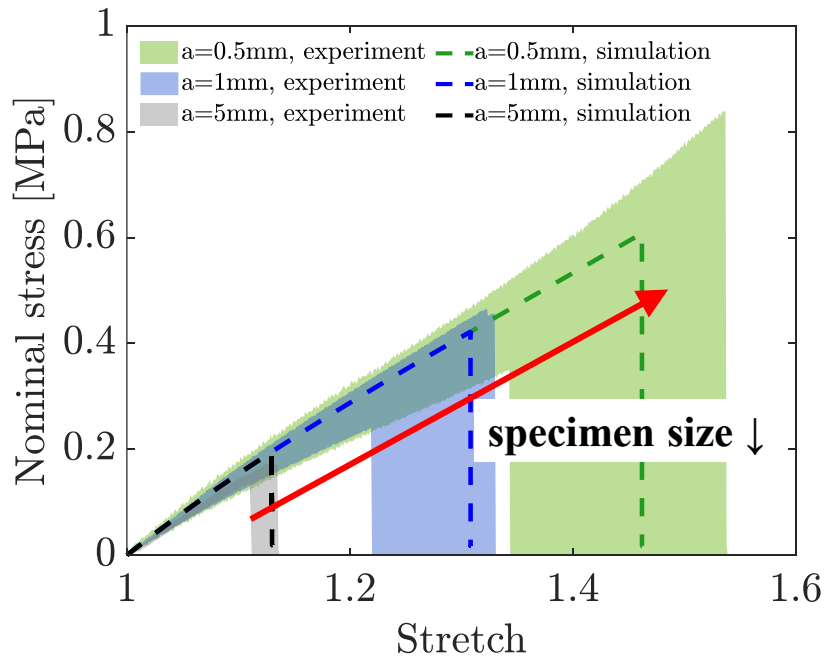# Results: Experiment vs. Numerical simulation[1]

- Strain fields in **TangoPlus** specimens ($l = 1mm$)

  - Larger specimen ruptures earlier
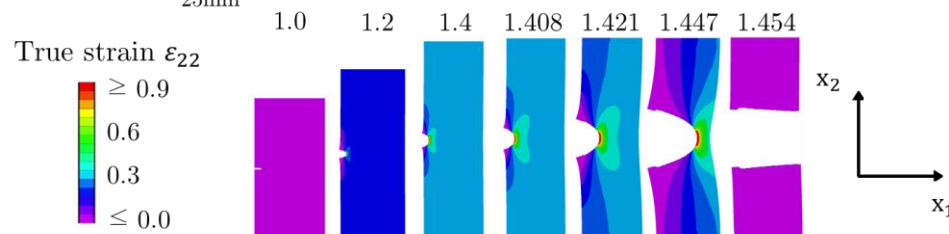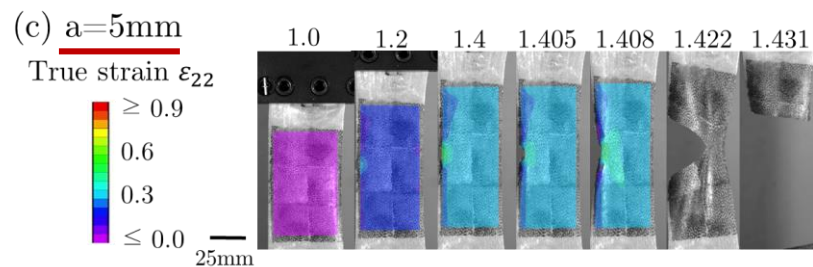
Results: Experiment vs. Numerical simulation[1]

- Notch lengths $a = \{0.5, 1, 5\}$ mm

- Geometric similarity $\rightarrow$ **Identical initial stress-stretch response**

- Smaller notch length $\rightarrow$ Higher rupture stretch

a) PDMS

b) TangoPlus
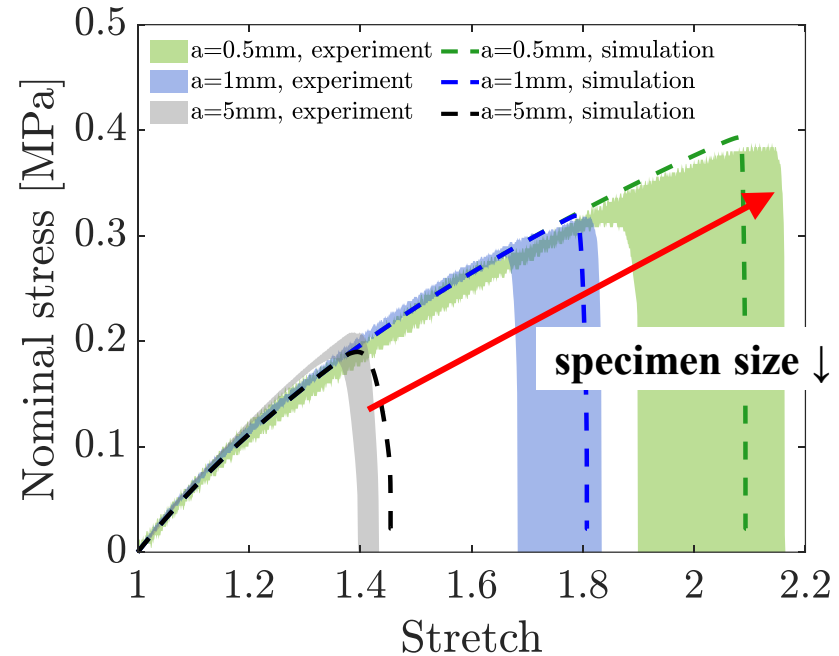
Notch-length sensitivity[1]

- PDMS vs. TangoPlus; same specimen sizes

  - PDMS: $l = 0.08mm$

  - TangoPlus: $l = 1mm$ $\Big\}$ **More than 10 times**

- Normalized rupture stretch

$$= \frac{\text{Rupture stretch of } \textbf{notched} \text{ specimens}}{\text{Rupture stretch of } \textbf{unnotched} \text{ specimens}}$$

- Normalized notch length $= \dfrac{\text{Notch length (a)}}{\text{Intrinsic length scale } (l)}$
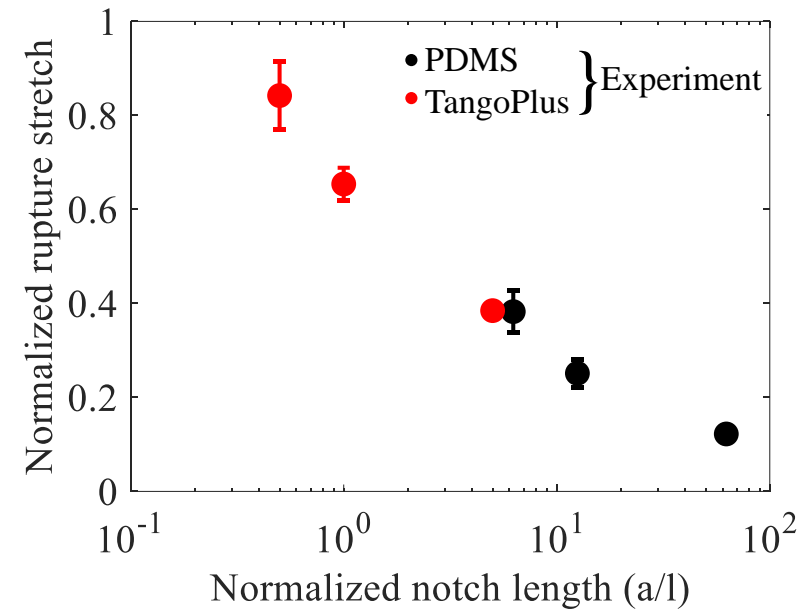
Notch-length sensitivity[1]

- PDMS vs. TangoPlus; same specimen sizes

  - PDMS: $l = 0.08mm$

  - TangoPlus: $l = 1mm$

  More than 10 times

- a/l: 0.5~5 (TangoPlus; $l = 1mm$) → Highly notch length-sensitive

- a/l: 5~50 (PDMS; $l = 0.08mm$) → Less notch length-sensitive
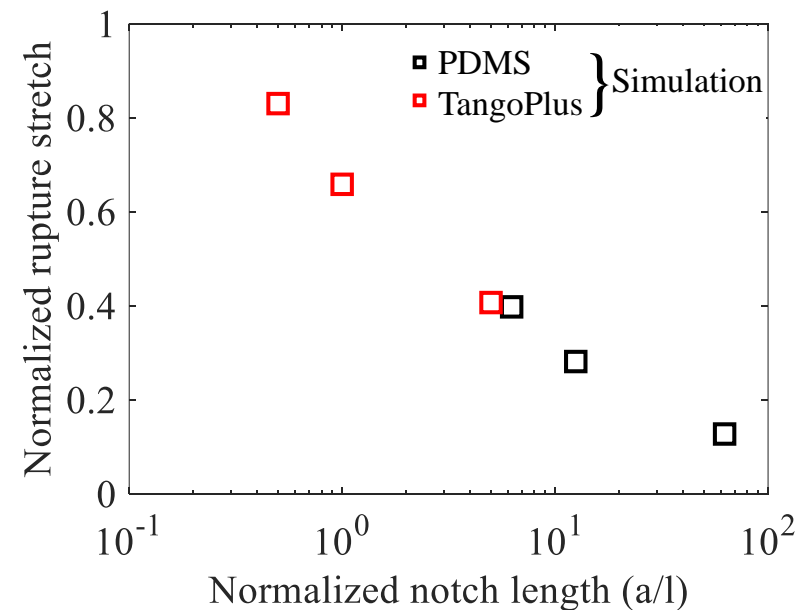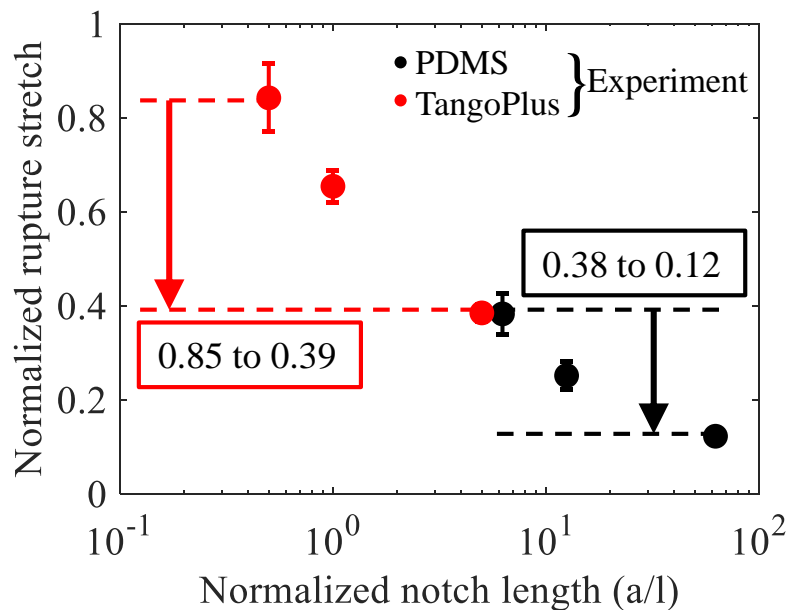
Randomly perforated specimen (TangoPlus)[1]

- Nicely predicted the response **without modification of parameters**
  - Progressive fracture of ligaments

(a) Experiment   Applied macroscopic stretch

True strain ε_{22}

(b) Simulation

True strain ε_{22}
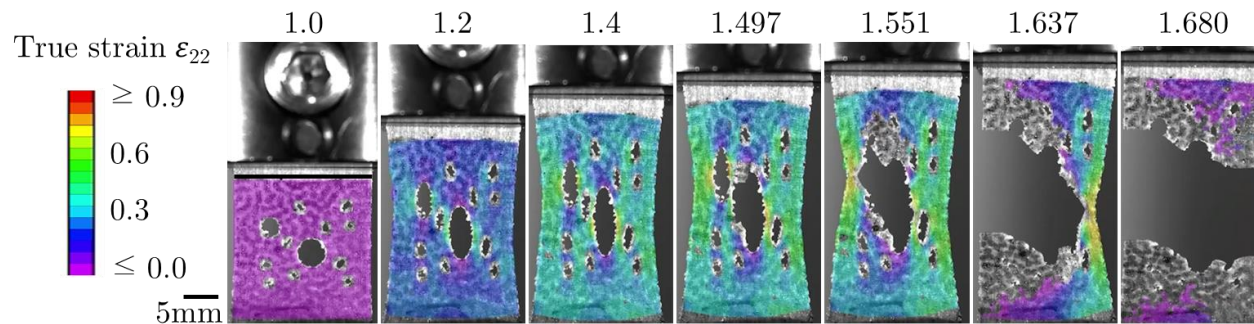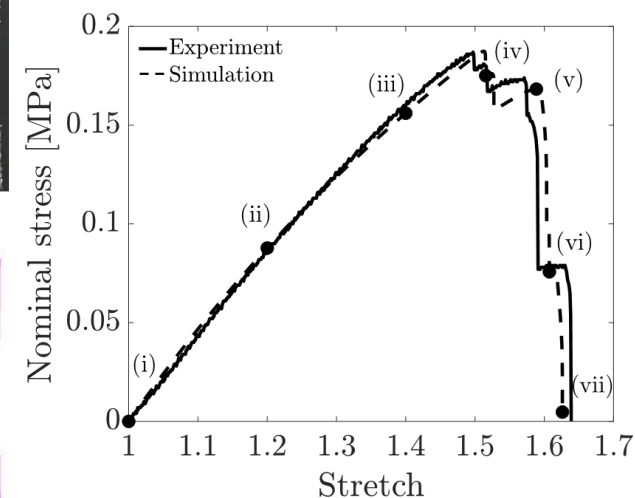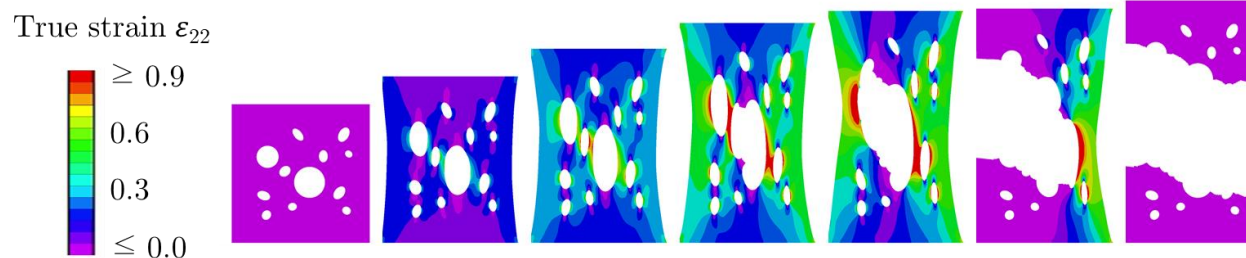
Conclusion

- **Size-dependent fracture** is clearly observed in experiments[1]

  - Rupture stretch increases as the notch length decreases

  - Size-dependence increases as the notch-root radius decreases

- **The intrinsic length scale** determines the size-dependent behavior[1]

  - The intrinsic length scale l defines the size of diffusive damage zone / fracture process zone

  - The intrinsic length scales were identified from experiments

  - Normalized notch length (a/l) determines the size-dependence

- **Nonlocal continuum model**[2,9] nicely predicted the fracture in elastomers[1]

  - Nonlocal continuum model utilizes experimentally identified intrinsic length scales

  - The model captures the size-dependent fracture in elastomers

  - The model is capable of predicting the fracture of complex geometries

Future work

- Fracture involving non-trivial dissipation
  - Mullins effect[16-20]

    → Is the fracture behavior influenced by the rate-independent dissipation (e.g., the Mullins effect) ?
  - Viscous dissipation[16-19,21]

    → How to describe complicated deformation and fracture behaviors in polymers?
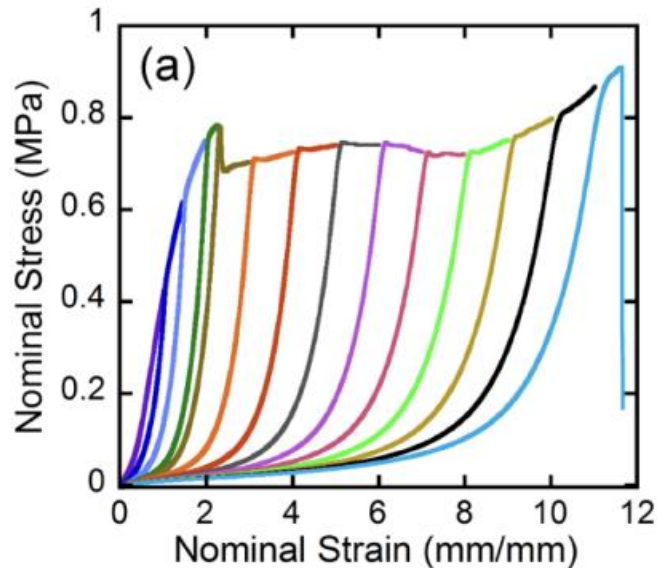
a) Fracture in double-network elastomers; the Mullins effect and fracture occur[20]
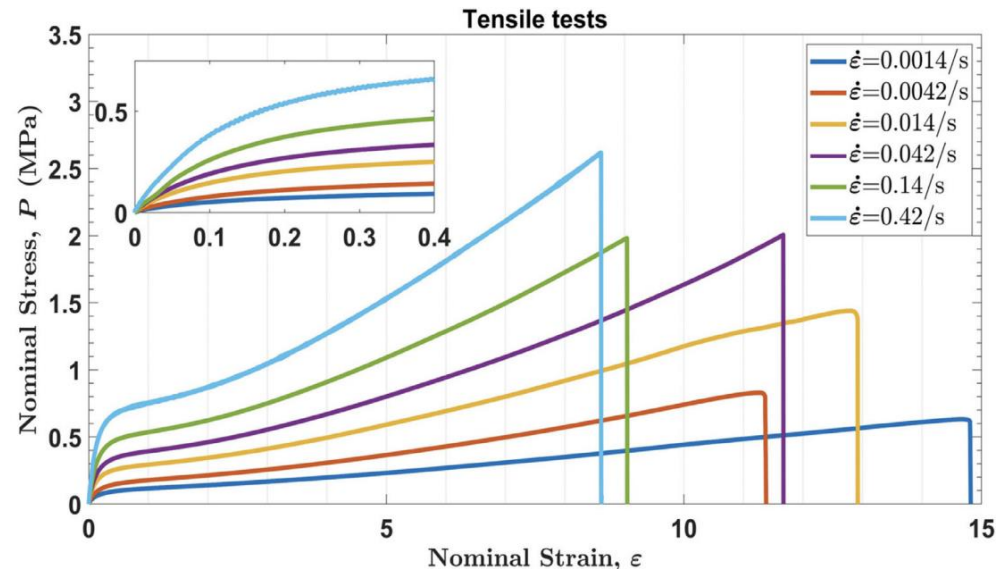
b) Rate-dependent deformation and fracture behaviors in a hydrogel (polyampholyte gel)[21]

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[21] Venkata, S. P., Cui, K., Guo, J., Zehnder, A. T., Gong, J. P., & Hui, C. Y. (2021). Constitutive modeling of bond breaking and healing kinetics of physical Polyampholyte (PA) gel. *Extreme Mechanics Letters, 43*, 101184.