Modelling the evolving ductility of biodegradable polymers

A. Hill[1], K.S. Bezela[1], R.N. Shirazi[1], M. Destrade[2], W. Ronan[1]

[1] Biomechanics Research Centre, Biomedical Engineering, NUI Galway
[2] School of Mathematics, Statistics and Applied Mathematics, NUI Galway

Postgraduate Modelling Research Group

email: a.hill5@nuigalway.ie

BioMEC

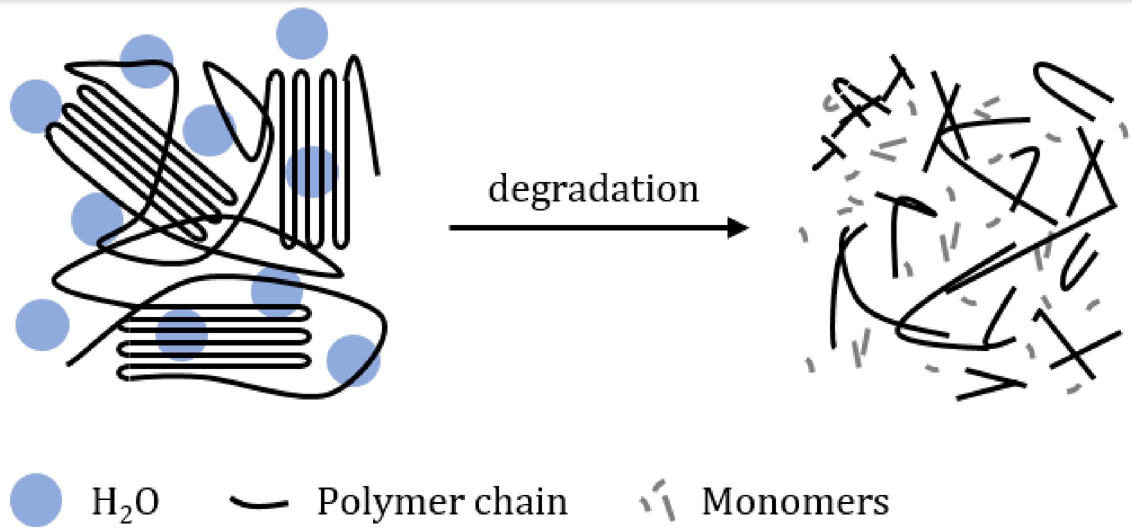
NUI Galway
OÉ Gaillimh

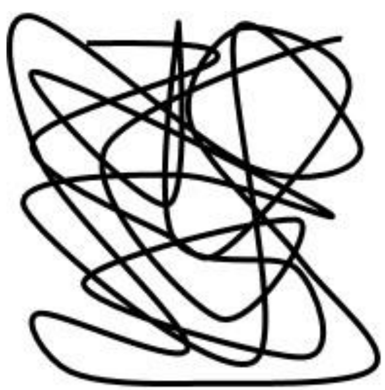
Research objective

- Develop a modelling framework for biodegradable polymers;
- For use in the medical device industry, specifically cardiovascular stents

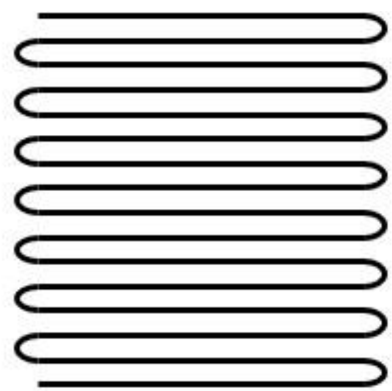
- Overcome risks associated with metal stents

Biodegradable polymers





Amorphous

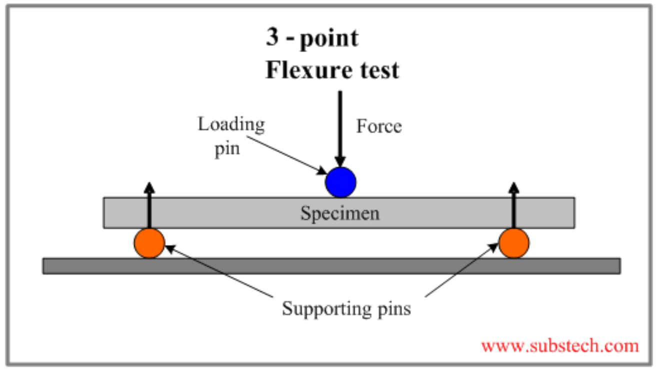


Crystalline

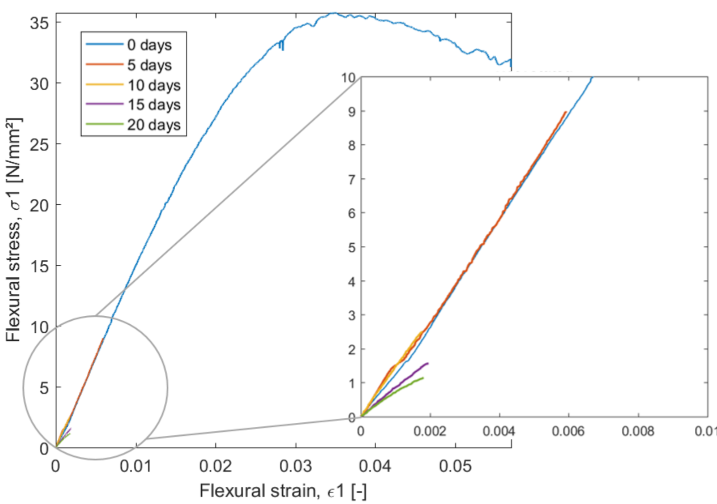
Semi-crystalline

Experimental observations

Ductile-to-brittle transition for increasing degradation duration in PLA:

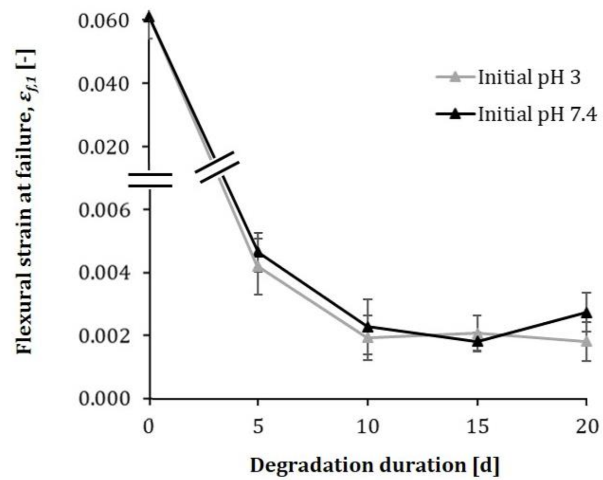


σ



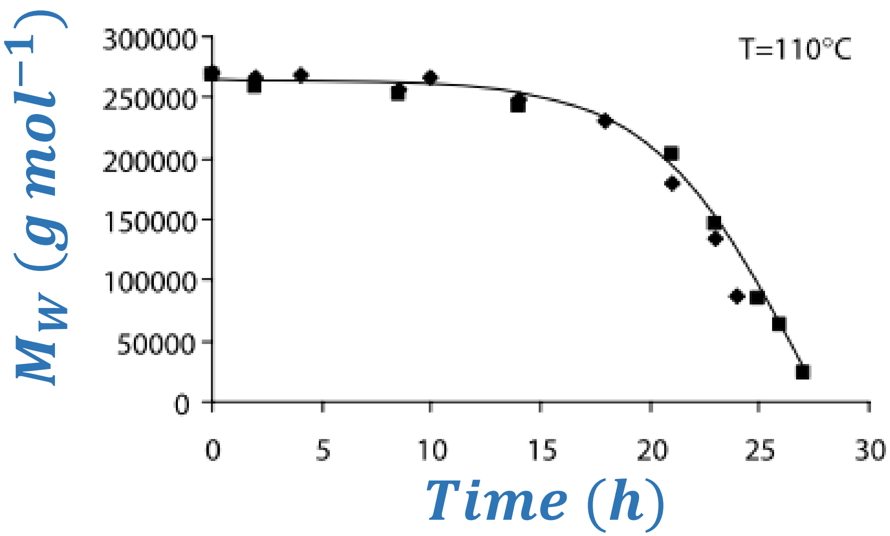
ε_f

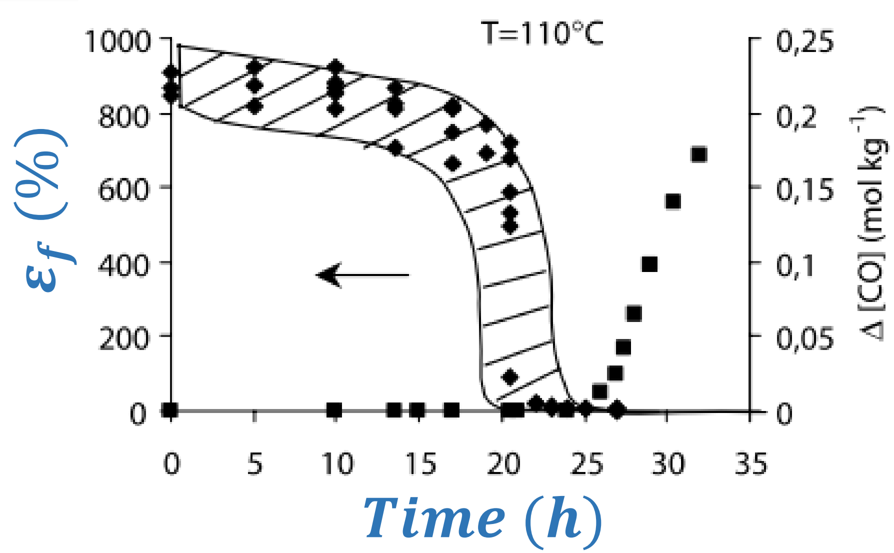
ε_f



time

Fayolle et al., 2004





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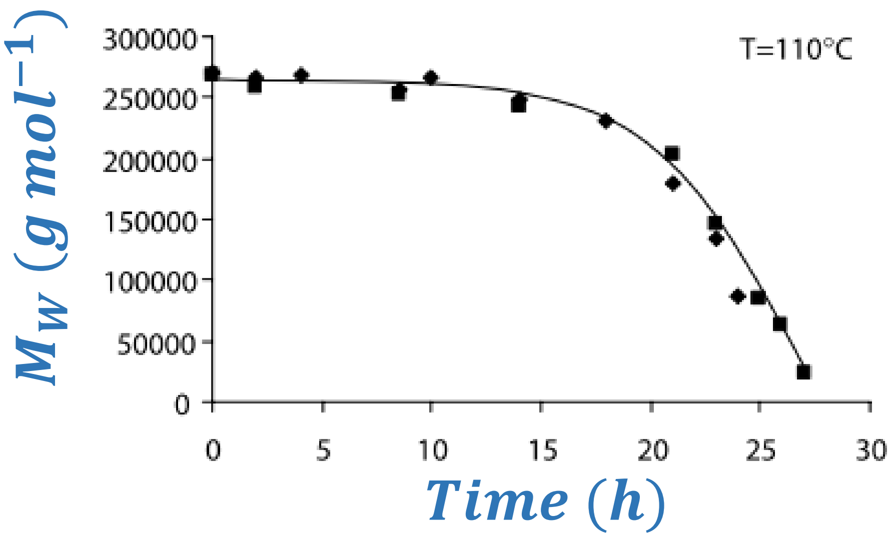
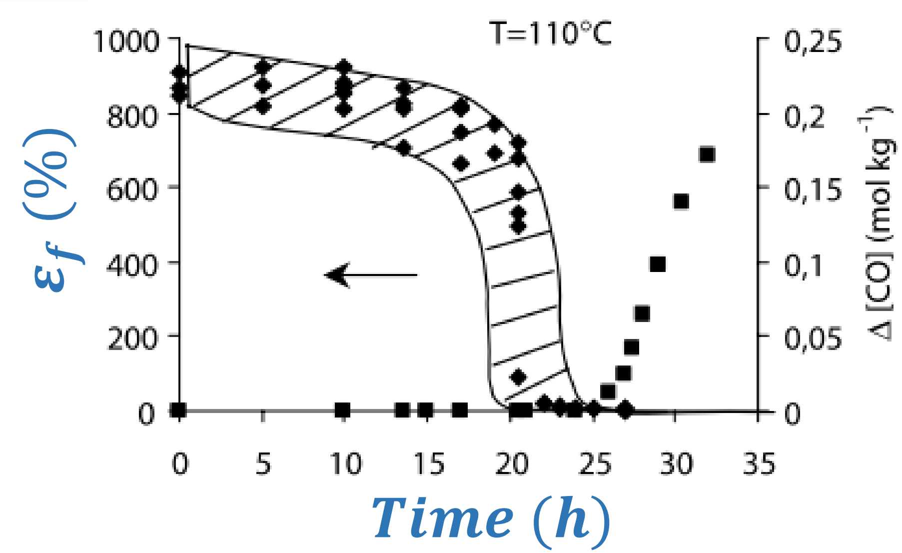
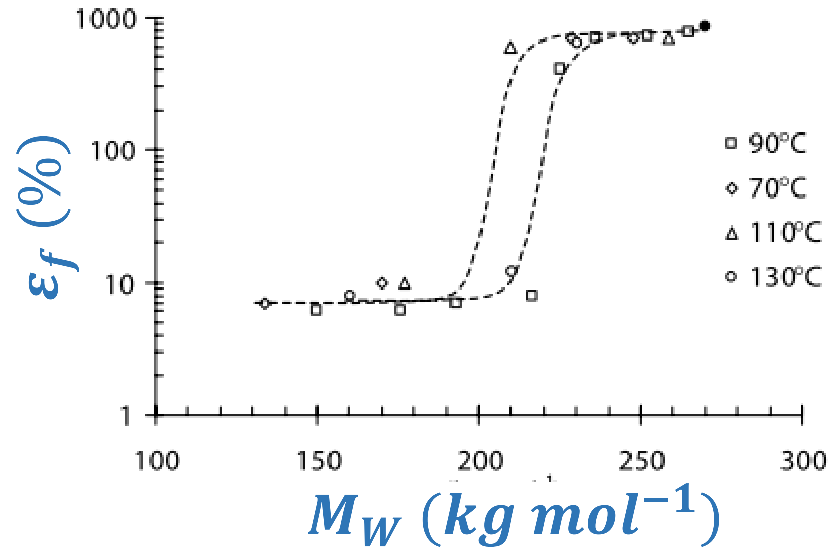
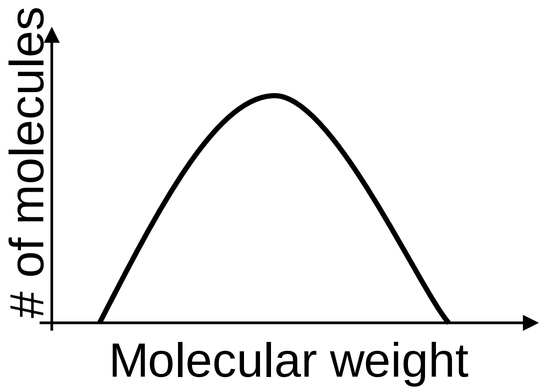


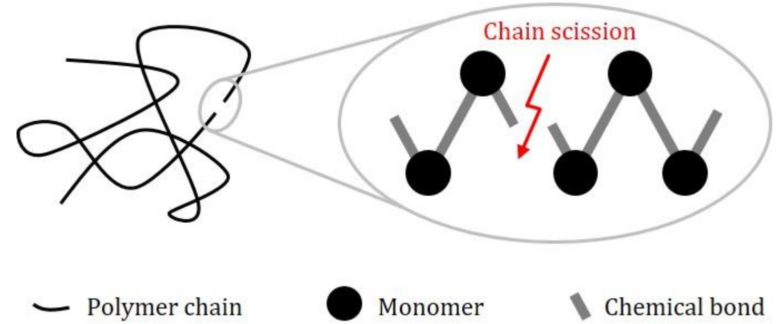




Current work

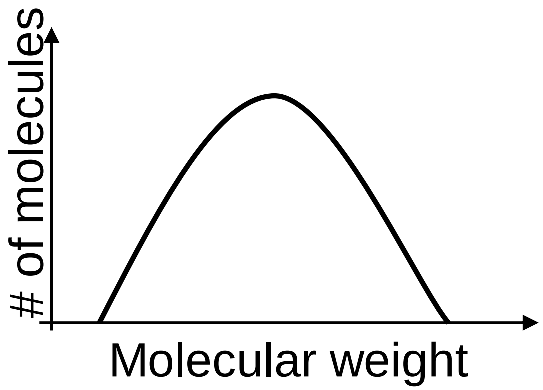


Degradation:



- End scissions
- Random scissions

Current work



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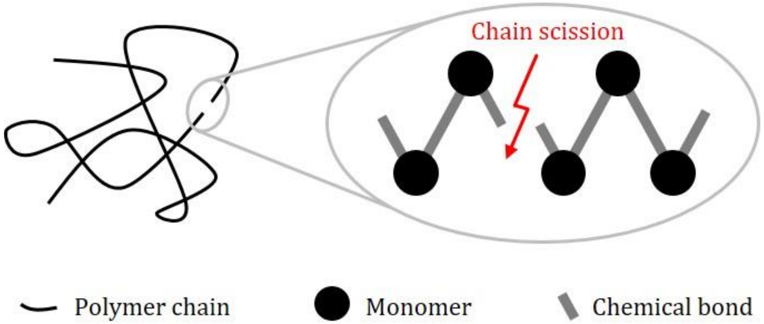
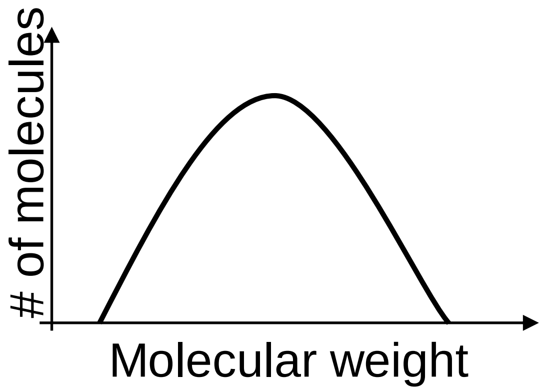


- End scissions
- Random scissions

Track chain lengths in MATLAB:

$$\left(\begin{array}{cccc} 1000 & 0 & 0 & \dots \\ 1020 & 0 & 0 & \dots \\ 1040 & 0 & 0 & \dots \\ 1060 & 0 & 0 & \dots \\ 1080 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \end{array}\right.$$

Current work



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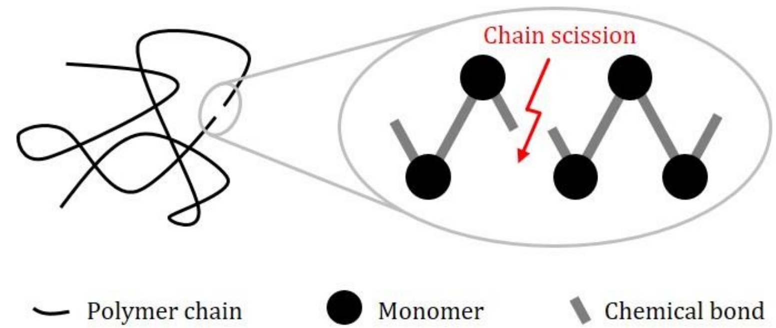

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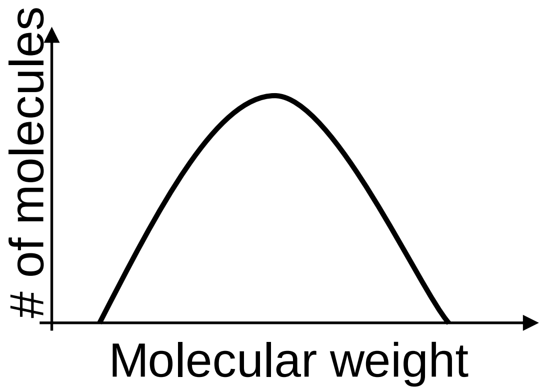

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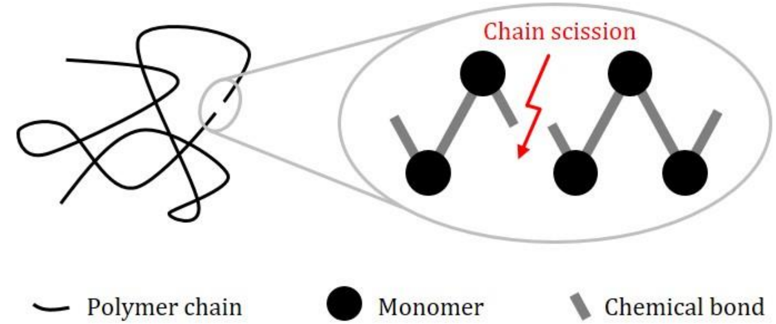
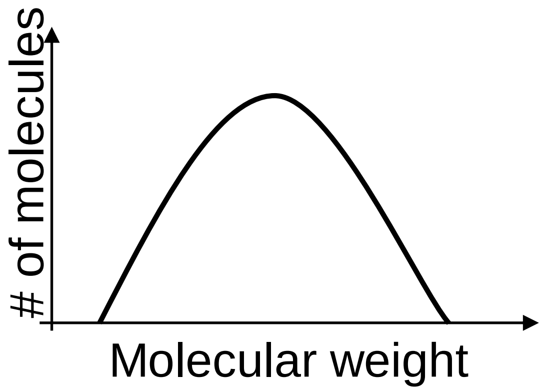


- End scissions
- Random scissions

Track chain lengths in MATLAB:

$$\left(\begin{array}{cccc} \mathbf{999} & 0 & 0 & \dots \\ 1020 & 0 & 0 & \dots \\ \mathbf{400} & \mathbf{640} & 0 & \dots \\ 1060 & 0 & 0 & \dots \\ 1080 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \end{array}\right.$$

Current work



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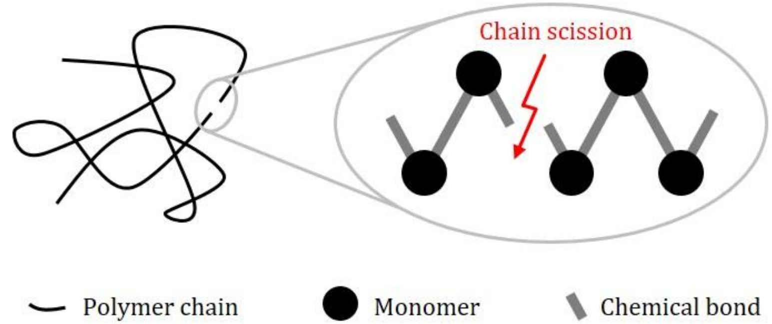
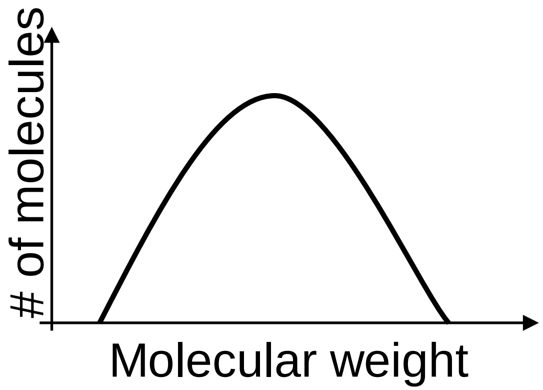


- End scissions
- Random scissions

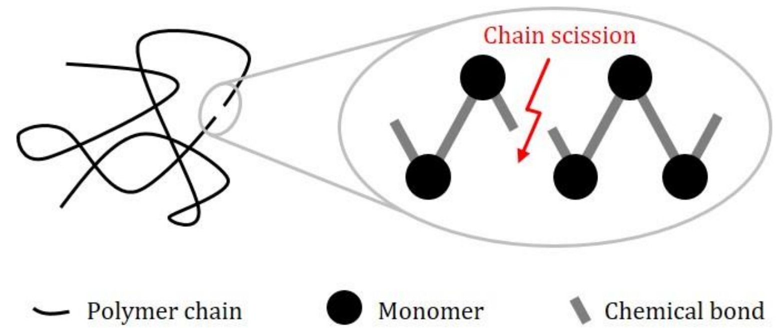
Track chain lengths in MATLAB:

$$
\begin{pmatrix}
999 & 0 & 0 & \dots \\
1020 & 0 & 0 & \dots \\
\color{red}{400} & 640 & 0 & \dots \\
1060 & 0 & 0 & \dots \\
\color{red}{1080} & 0 & 0 & \dots \\
\vdots & \vdots & \vdots &
\end{pmatrix}
$$

Current work



Degradation:

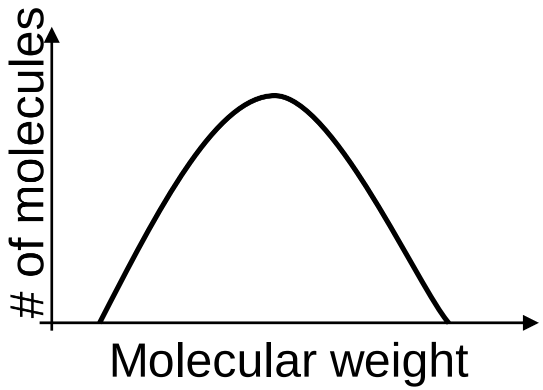


- End scissions
- Random scissions

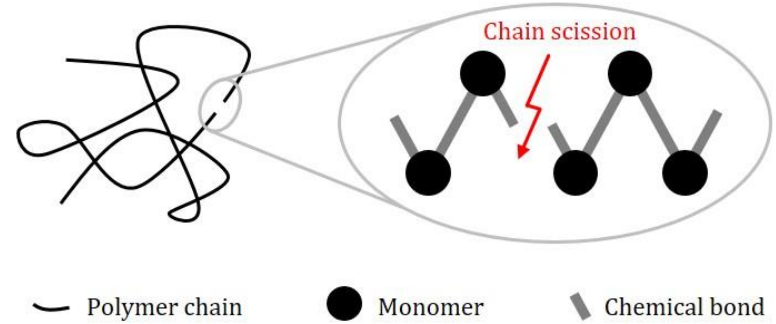
Track chain lengths in MATLAB:

$$\left(\begin{array}{rccc} 999 & 0 & 0 & \dots \\ 1020 & 0 & 0 & \dots \\ \mathbf{398} & 640 & \mathbf{2} & \dots \\ 1060 & 0 & 0 & \dots \\ \mathbf{1079} & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \end{array} \right.$$

Current work



Degradation:



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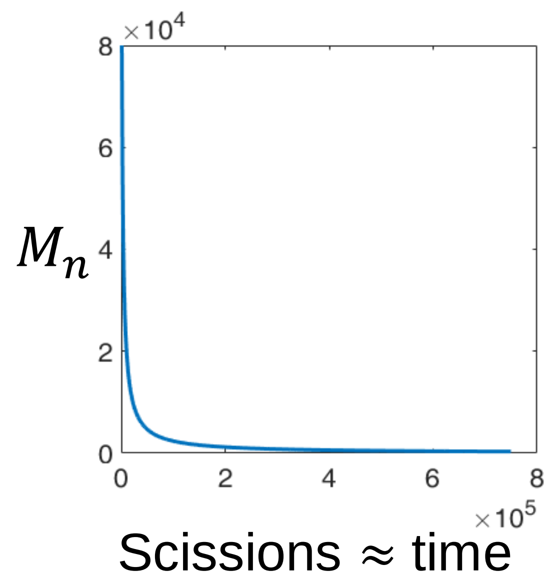
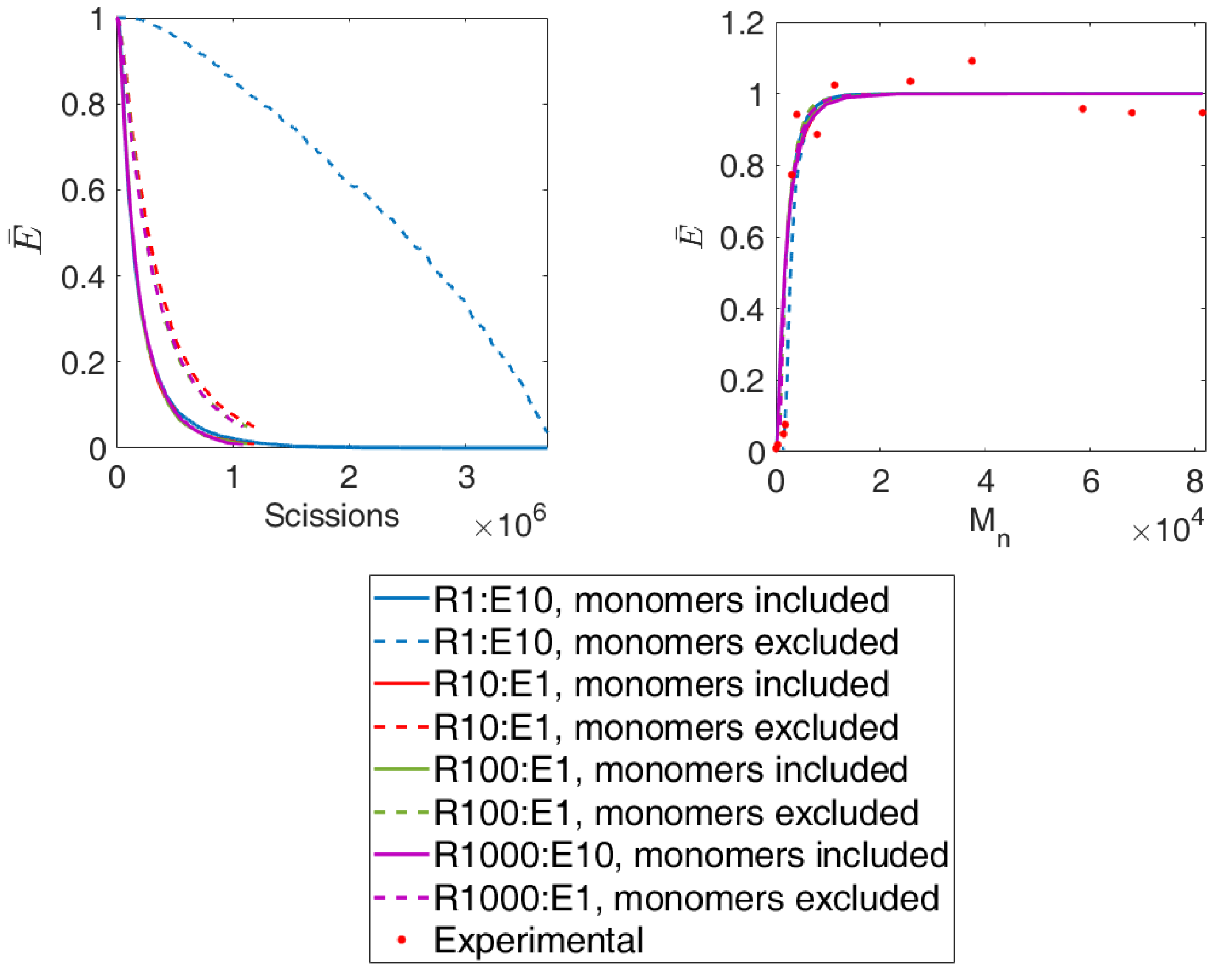


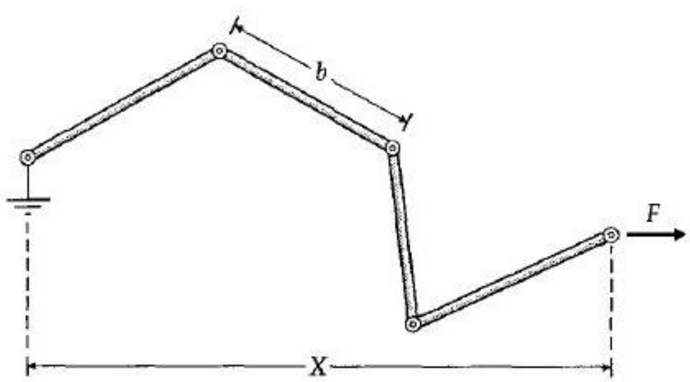
Predicted stiffness



Relating strain failure to polymer units

Freely jointed chain:

- Behaves as entropic spring



$\varepsilon_f^{M_n}$ - related to M_n

ε_f^{N} - related to chains above M_n^{crit}

Maximum length of extended chain before failure, $L_f = N$

Root mean-square end-to-end distance, $\sqrt{N} = L_0$

Strain failure, ε_f:

Engineering strain:

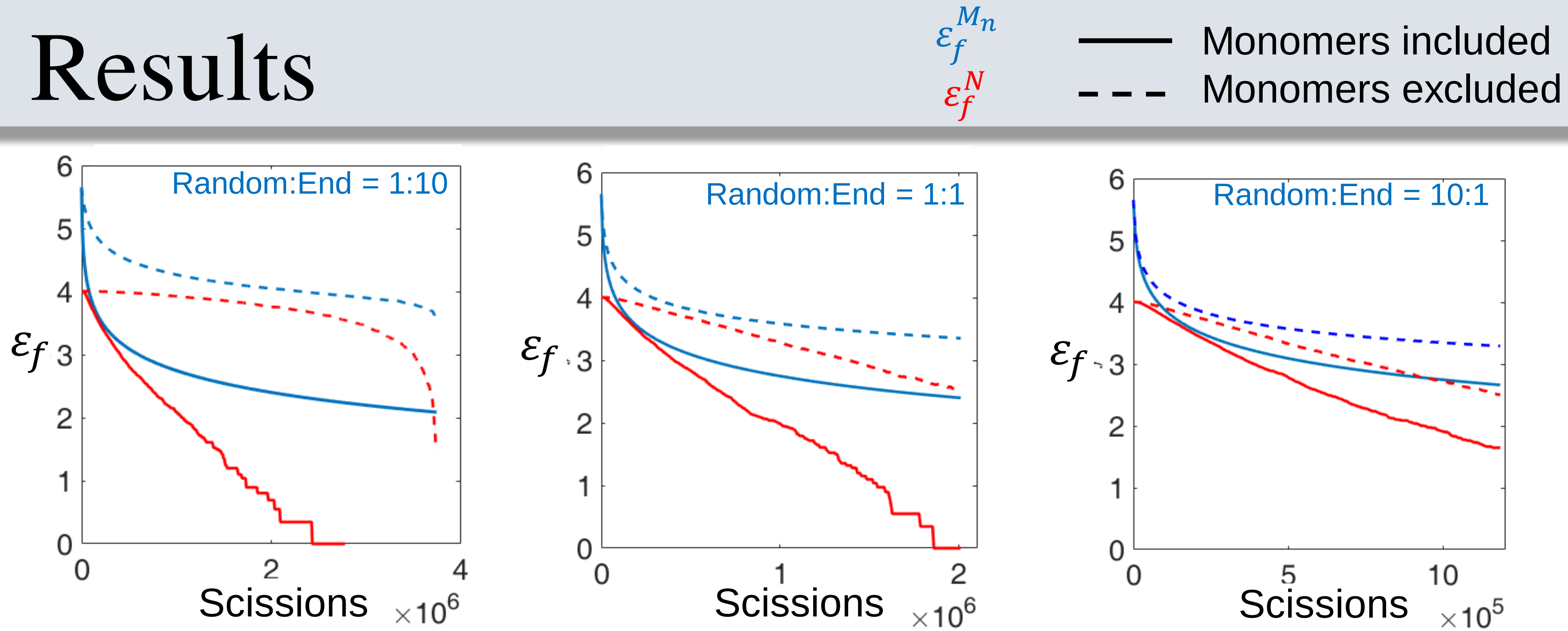
$$e_f = \frac{L_f - L_0}{L_0} = \frac{N - N^{\frac{1}{2}}}{N^{\frac{1}{2}}} = N^{\frac{1}{2}} - 1$$

True strain:

$$\varepsilon_f = \ln(1 + e_f) = \frac{1}{2}\ln(N)$$

N = number of polymer units

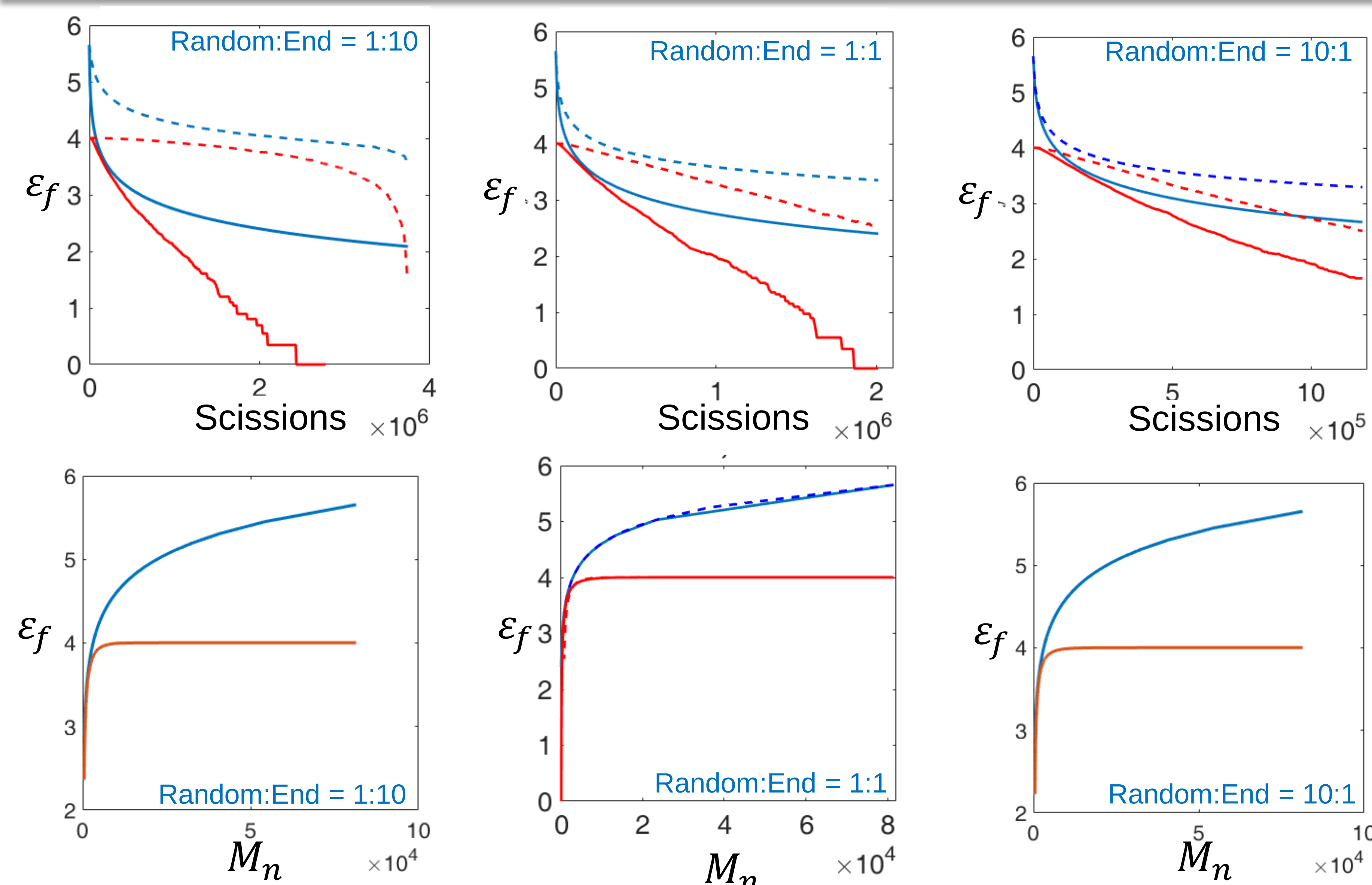
Results



$\varepsilon_f^{M_n}$
ε_f^{N}
Monomers included
Monomers excluded
Random:End = 1:10
Random:End = 1:1
Random:End = 10:1
ε_f
Scissions
$\times 10^6$
$\times 10^5$

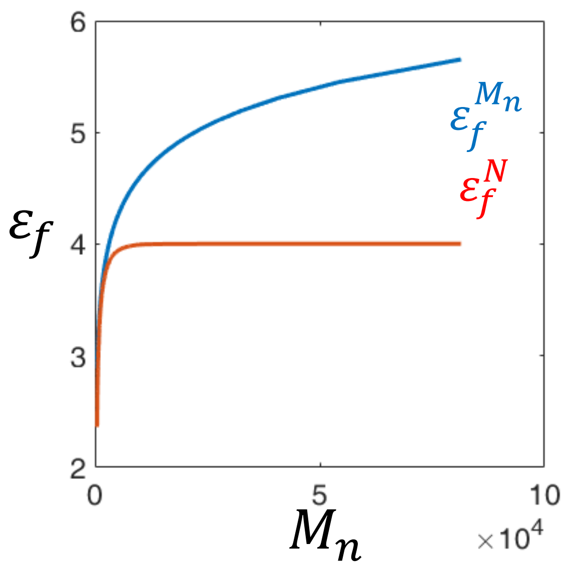
Results

$\varepsilon_f^{M_n}$ ε_f^{N} Monomers included Monomers excluded

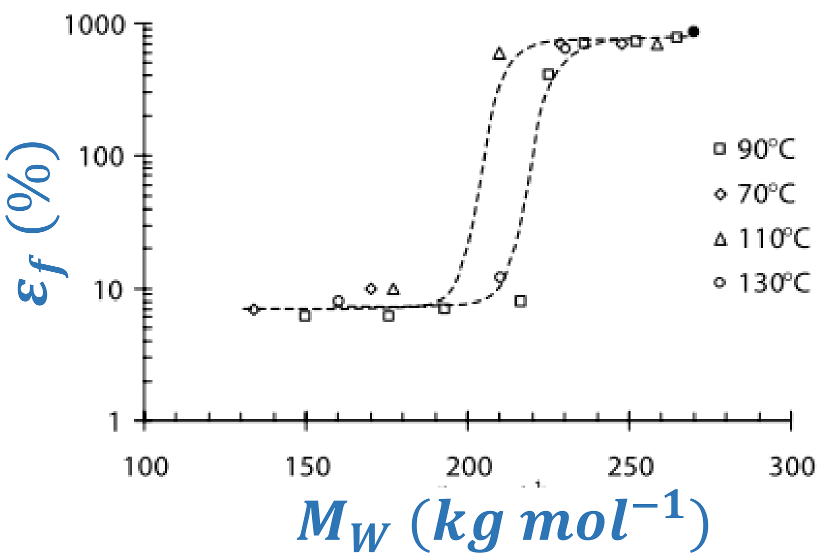


Comparing results

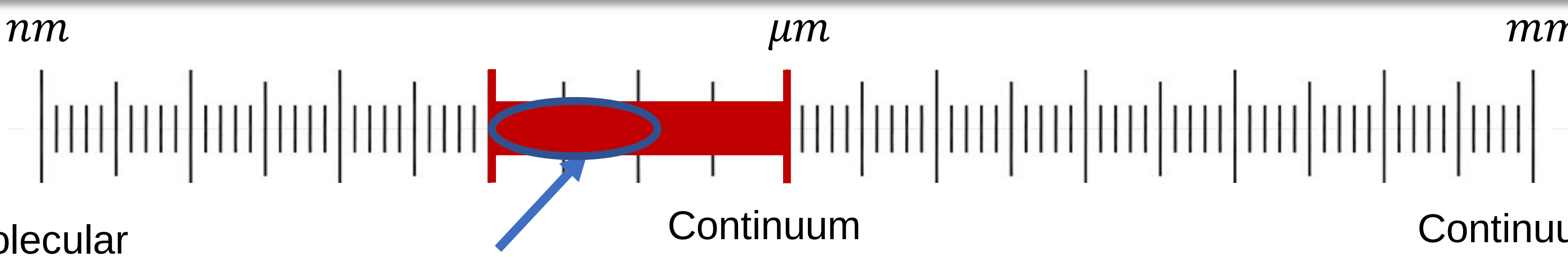
Current results:



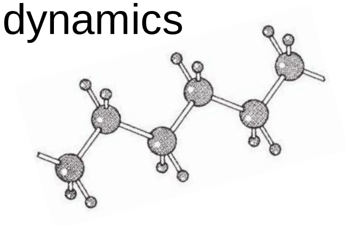
Fayolle et al., 2004:



Further work



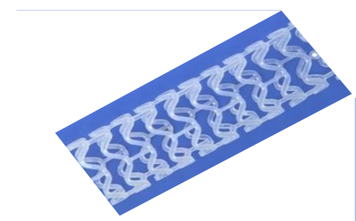
Molecular dynamics



Area of interest

Continuum material models

Continuum device models



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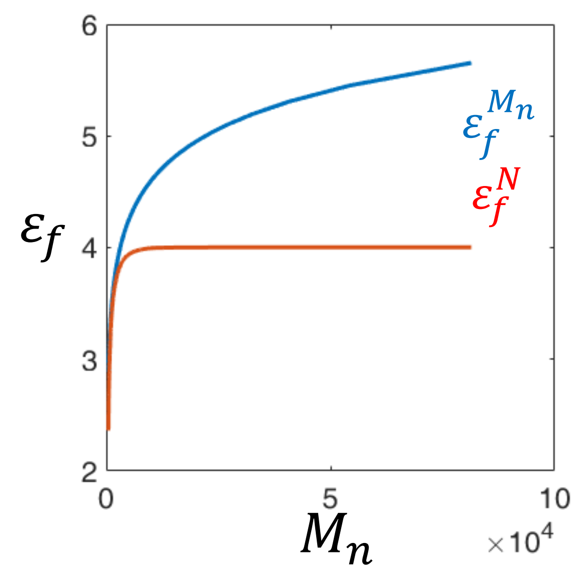
Wang et al., 2008:

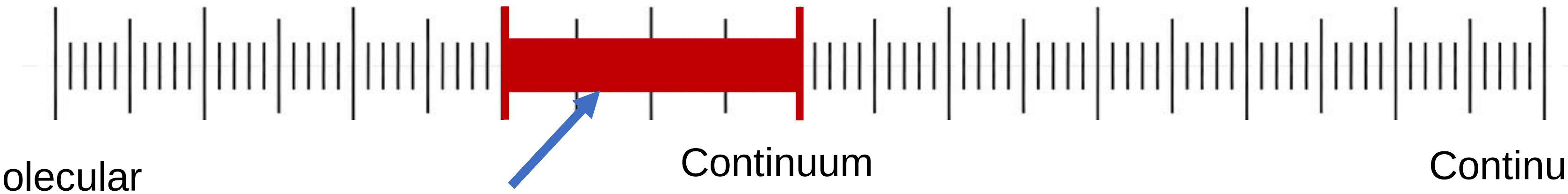
$$\frac{\partial M_n}{\partial t} = -\left(k_1 M_n + k_2 M_n C_m^\beta\right)$$

$$\frac{\partial C_m}{\partial t} = k_1 M_n + k_2 M_n C_m^\beta + \nabla \cdot (D \nabla C_m)$$



Further work

nm μm mm



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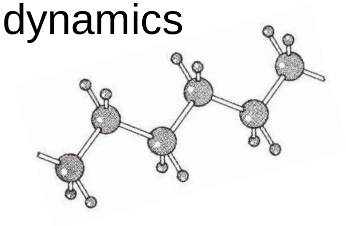

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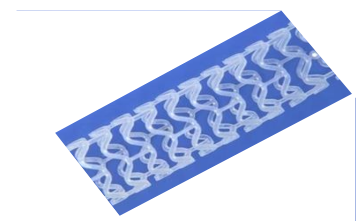

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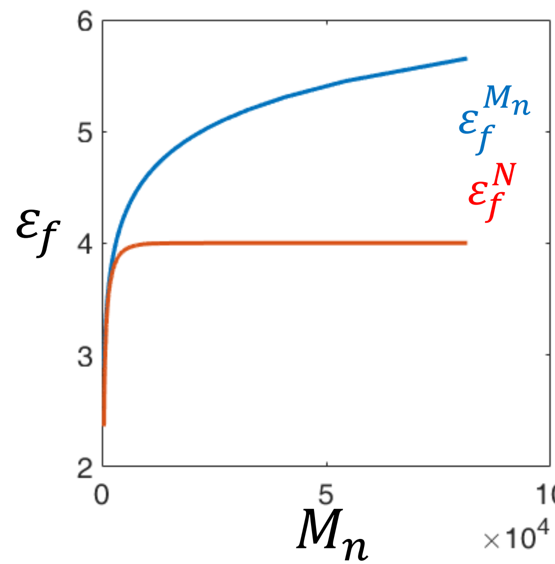

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