A Multiscale Cohesive Zone Model for Rate Dependent Fracture of Interfaces

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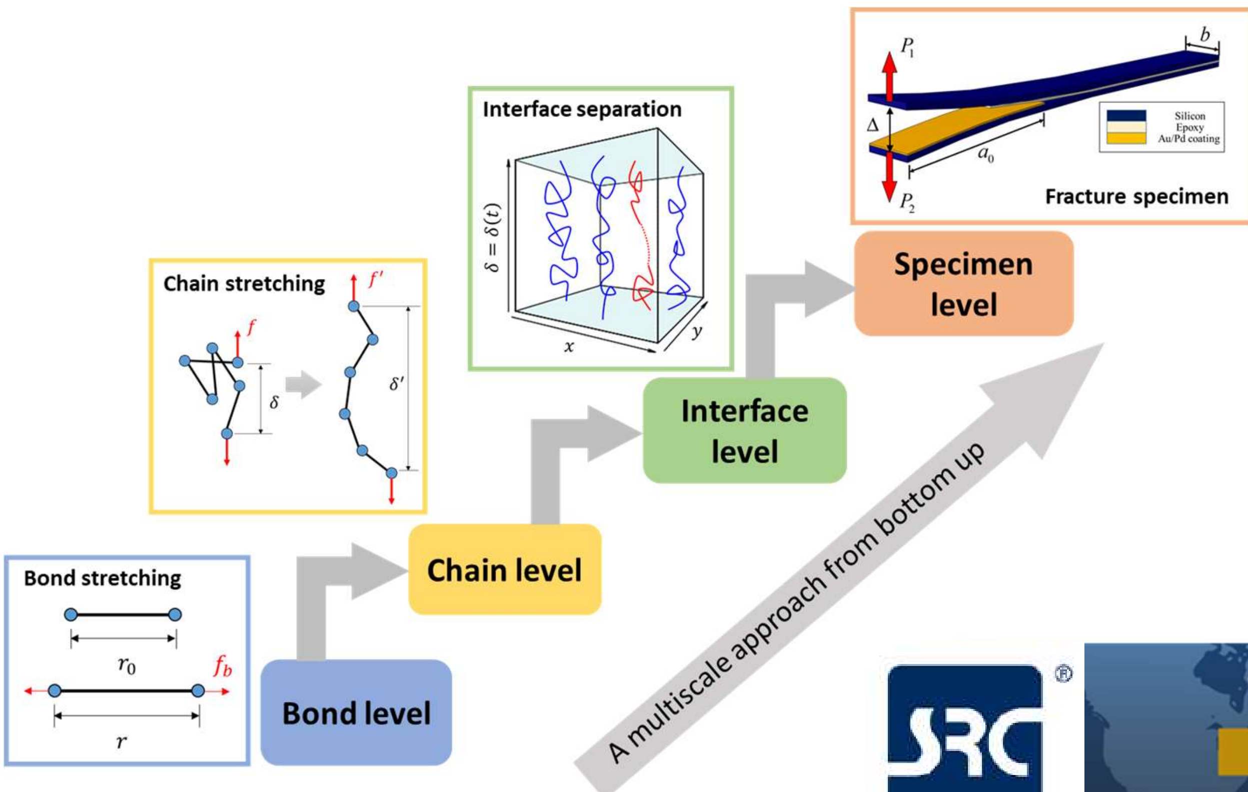
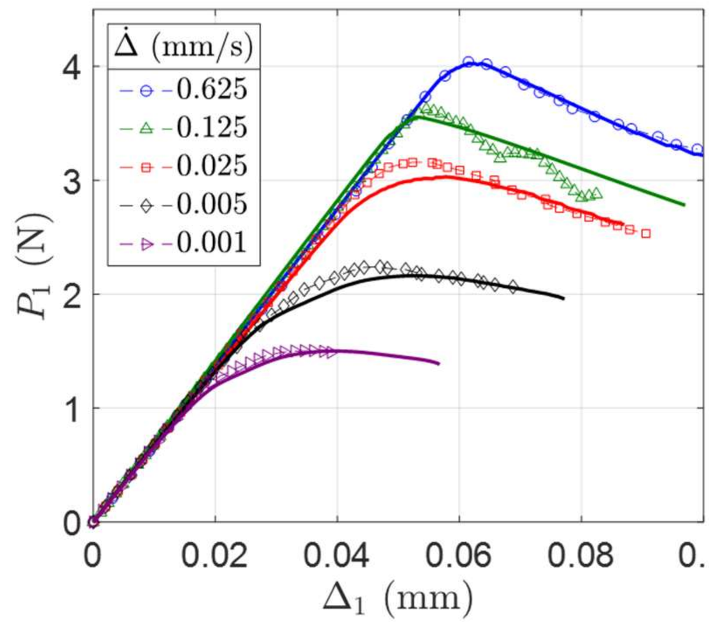
J. Mech. Phys. Solids 145, 104142 (2020).

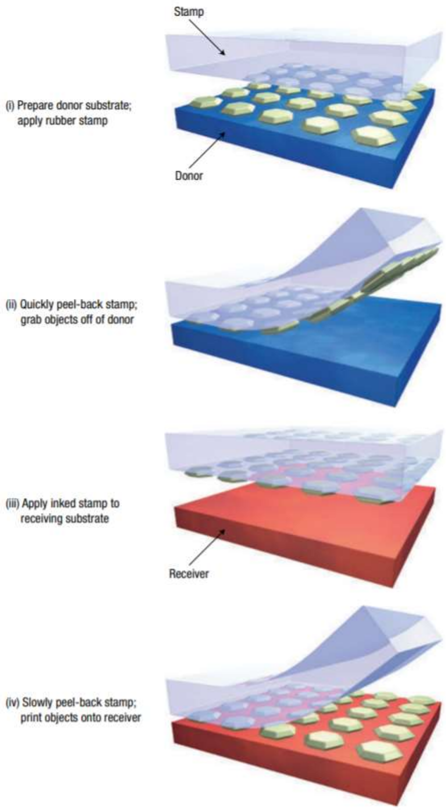
Congratulations Ravi!

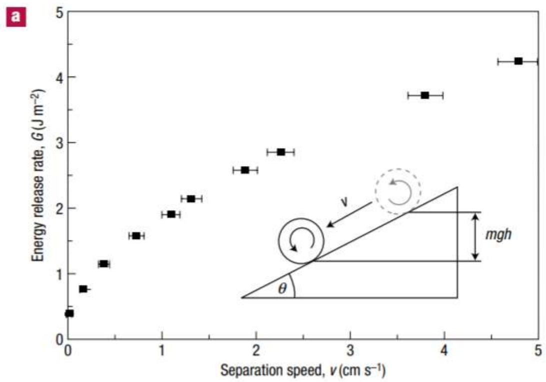


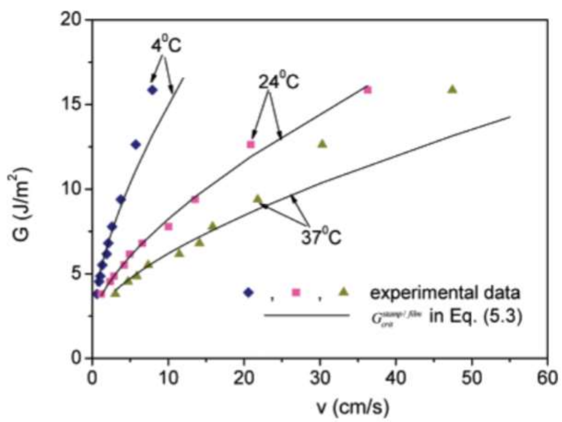


Rate-dependent fracture of interfaces

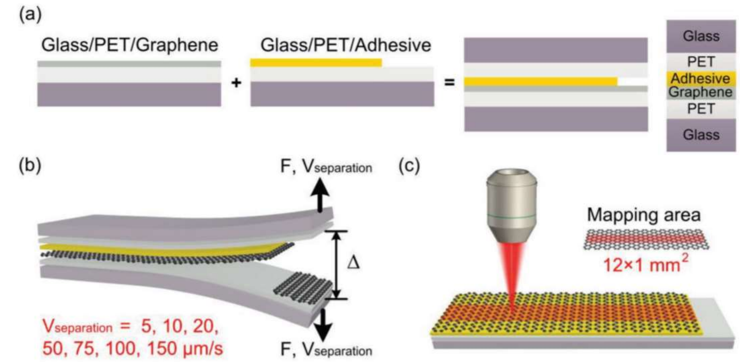
Kinetically Controlled Transfer Printing (Meitl et al., 2006; Feng et al., 2007)

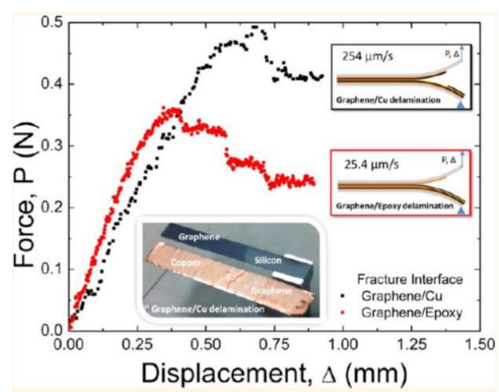


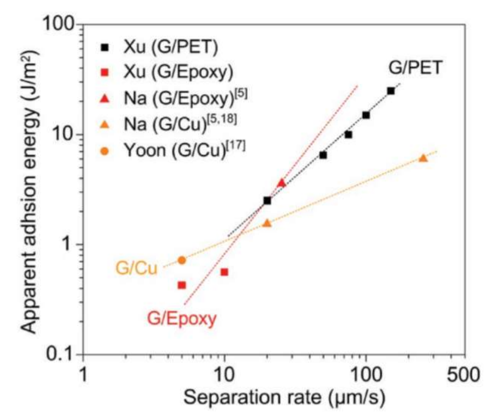




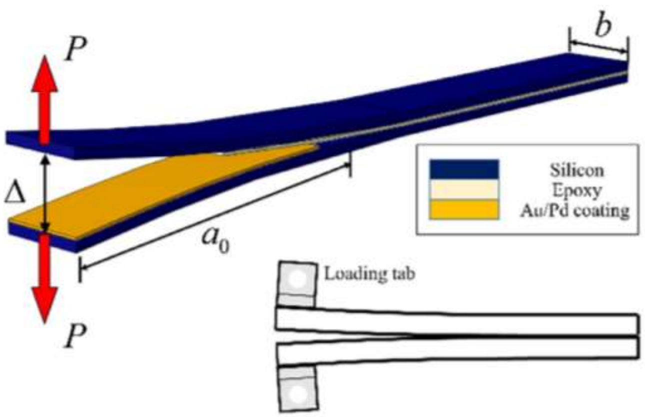
Selective dry transfer of graphene (Na et al., 2015; Xu et al., 2019)

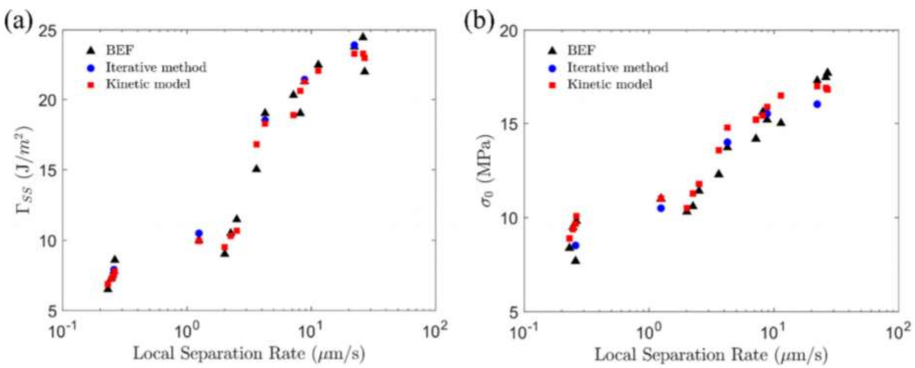


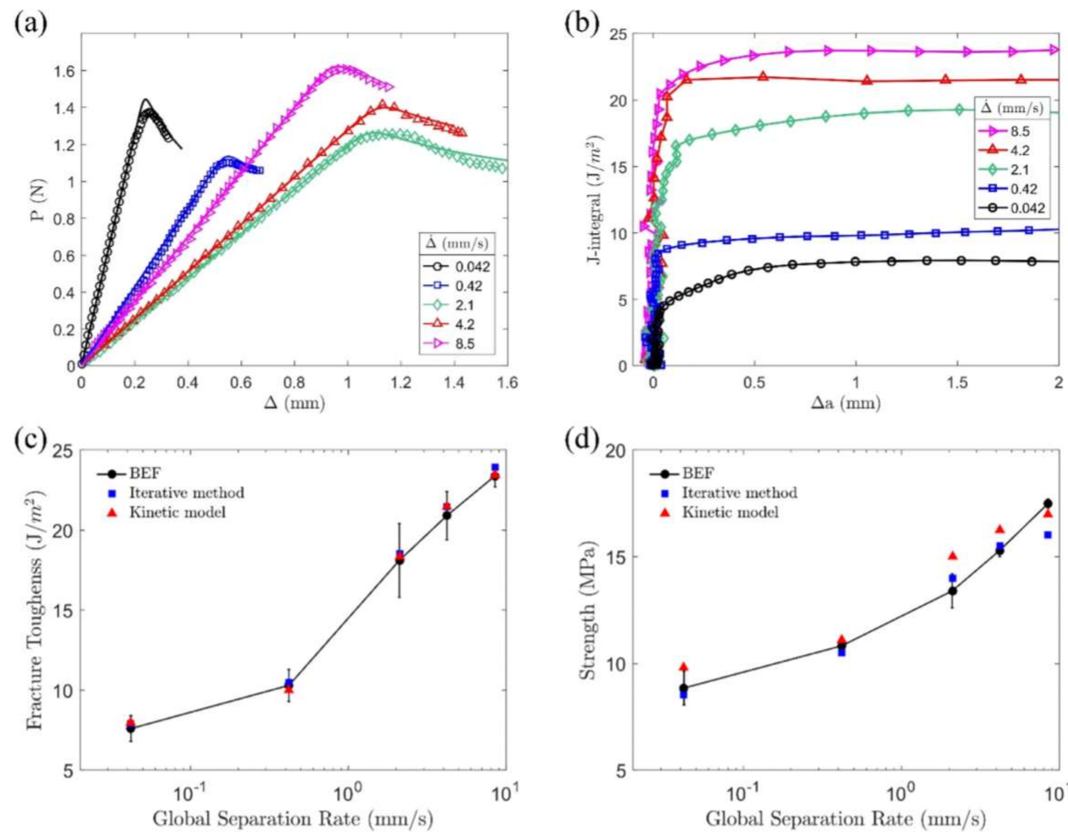




Rate-dependent fracture of a silicon/epoxy interface



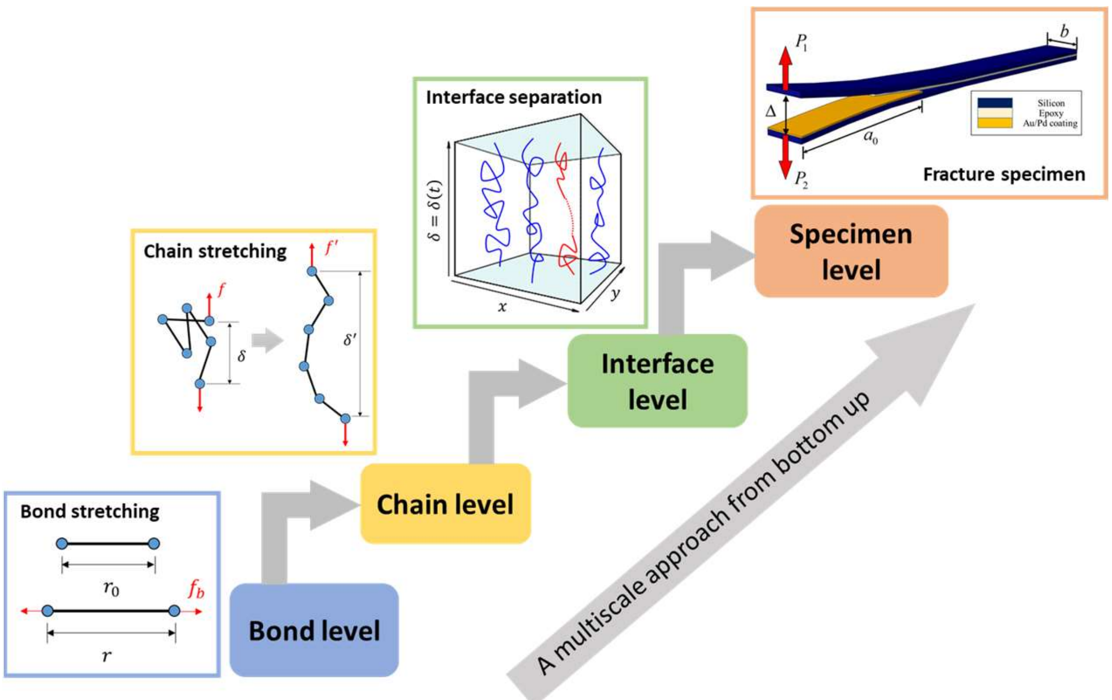




Hypothesis: toughness/strength depend on the local separation rate.

T. Yang, et al., J. Mech. Phys. Solids 131, 1-19 (2019).

A multiscale modeling approach



- Interfacial traction and separation:

$$\delta = \lambda_n n r_0$$

$$\sigma = \int (1 - D_n)\rho_0(n) f(\lambda_n) dn$$

- Damage evolution (thermally activated):

$$\frac{dD_n}{dt} = \frac{n}{t_0}(1 - D_n)\exp\left(-\frac{E_b}{k_B T}\right)$$

- An energy barrier:

$$E_b = E_b(f) \text{ or } E_b(\lambda_n)$$

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Bond model (Kuhn segment)

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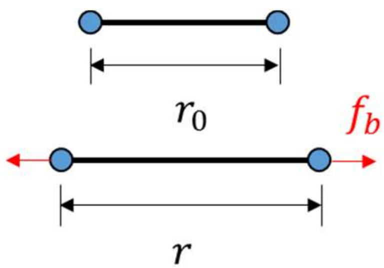

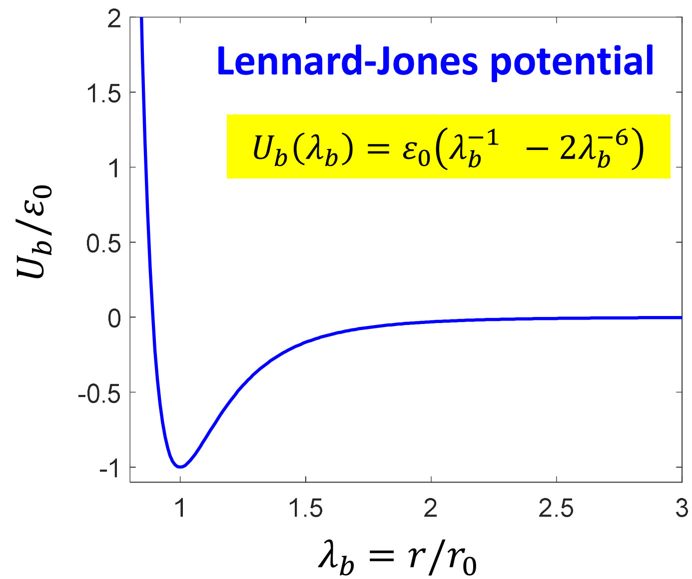

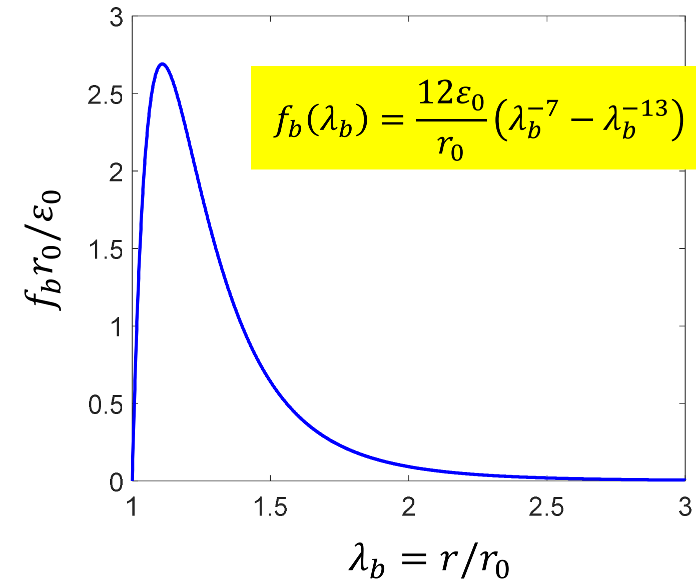

2 bond parameters:

$r_0 \rightarrow$ equilibrium bond length

$\varepsilon_0 \rightarrow$ bond energy

3 key features for a simple bond model:

(1) The potential energy is minimized at an equilibrium bond length;

(2) The potential energy becomes infinitely high as the two atoms approach each other;

(3) The potential energy approaches zero as the two atoms are separated far apart from each other.

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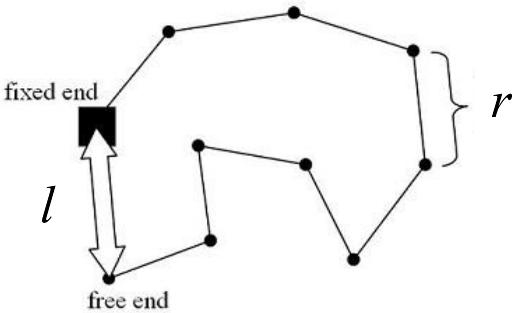
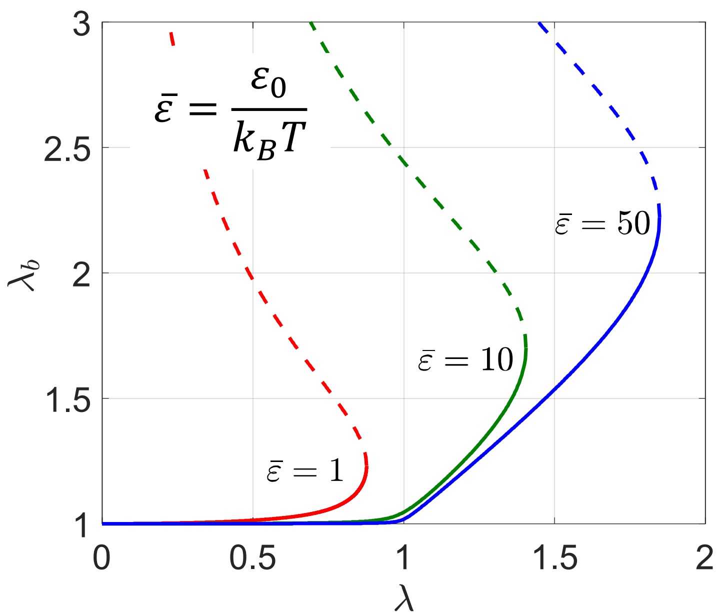
Chain model

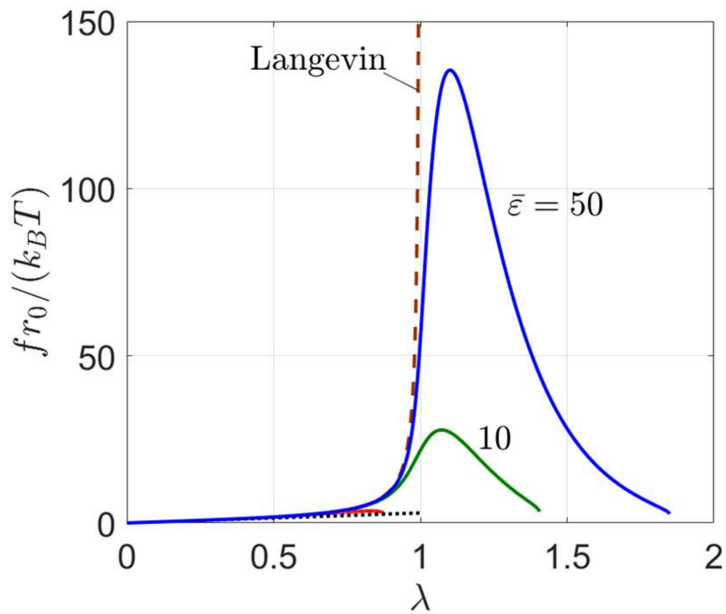
A freely jointed chain with stretchable bonds



$$\psi(\lambda,\lambda_b) = nU_b(\lambda_b) + nk_BT\left(\beta\mathcal{L}(\beta) + \ln\left(\frac{\beta}{\sinh\beta}\right)\right) \Rightarrow \frac{fr_0}{k_BT} = \bar{f}(\lambda,\bar{\varepsilon})$$

$$\lambda_b = \frac{r}{r_0} \qquad \lambda = \frac{l}{nr_0} \qquad \beta = \mathcal{L}^{-1}\left(\frac{\lambda}{\lambda_b}\right) \qquad \mathcal{L}(\beta) = \coth(\beta) - \beta^{-1}$$





The chain stretch transitions from linear (Gaussian) to nonlinear and from ***entropic*** to ***enthalpic***, with a peak force and a peak stretch.

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Kinetics of thermally activated chain scission

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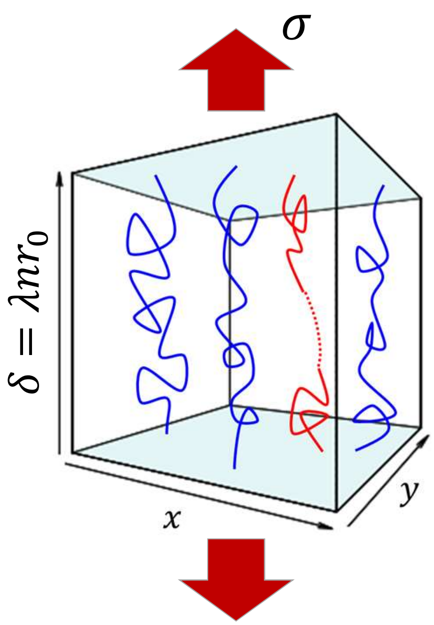

$$\sigma = Nf = (1 - D)N_0 f(\delta)$$

Assume a constant chain length (n) for now.

- **Bond survival probability** $R_b = N/N_0$

$$\frac{\dot{R}_b}{R_b} = -\frac{1}{t_0}\exp\left(-\frac{E_b}{k_B T}\right)$$

- **Chain survival probability** $R_{chain} = R_b^n$

$$\frac{\dot{R}_{chain}}{R_{chain}} = -\frac{n}{t_0}\exp\left(-\frac{E_b}{k_B T}\right)$$

- **Damage evolution** $D = 1 - R_{chain}$

$$\frac{dD}{dt} = \frac{n}{t_0}(1 - D)\exp\left(-\frac{E_b}{k_B T}\right)$$

What is the activation energy or energy barrier?

A microscopic time scale: $t_0 \sim \frac{\hbar}{k_B T} \sim 10^{-13}$ s

Is this relevant?

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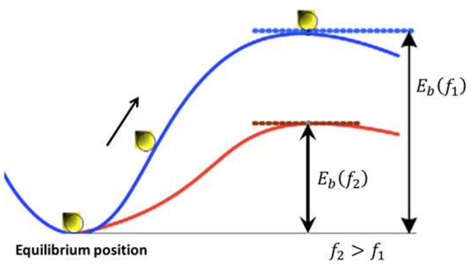
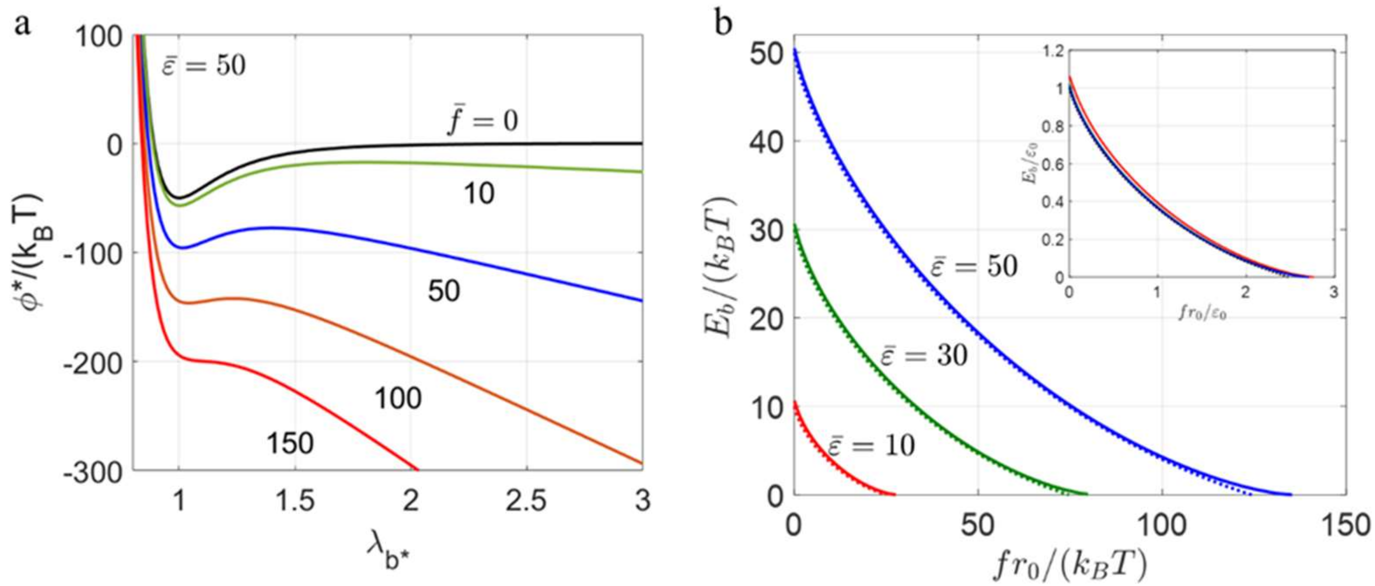
Energy barrier for chain scission



Transition-state theory: The transition from an equilibrium state of the chain to the state of a broken chain (with one broken bond) may be traversed along a path with the minimum energy barrier in the energy landscape.



$$E_b = \phi^*_{max} - \phi^*_{mi} \approx \varepsilon_0\left(1 - 1.664\hat{f}^{6/7} + \hat{f} + 0.0236\hat{f}^2\right)$$

$$\hat{f} = \frac{fr_0}{\varepsilon_0}$$

- An external force lowers the energy barrier (nonlinearly) for chain scission.
- The energy barrier becomes zero at the peak force for each chain.
- Reverse transition (healing) is possible under displacement control.

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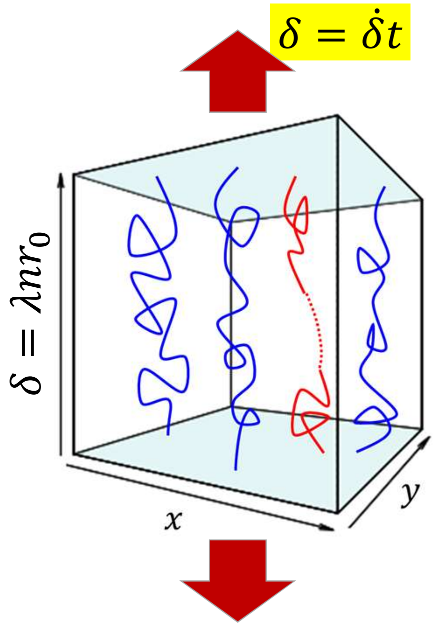
Rate-dependent traction-separation relations



$$\bar{\sigma} = \frac{\sigma r_0}{N_0 k_B T}$$

$$\bar{\delta} = \frac{\delta}{n r_0}$$

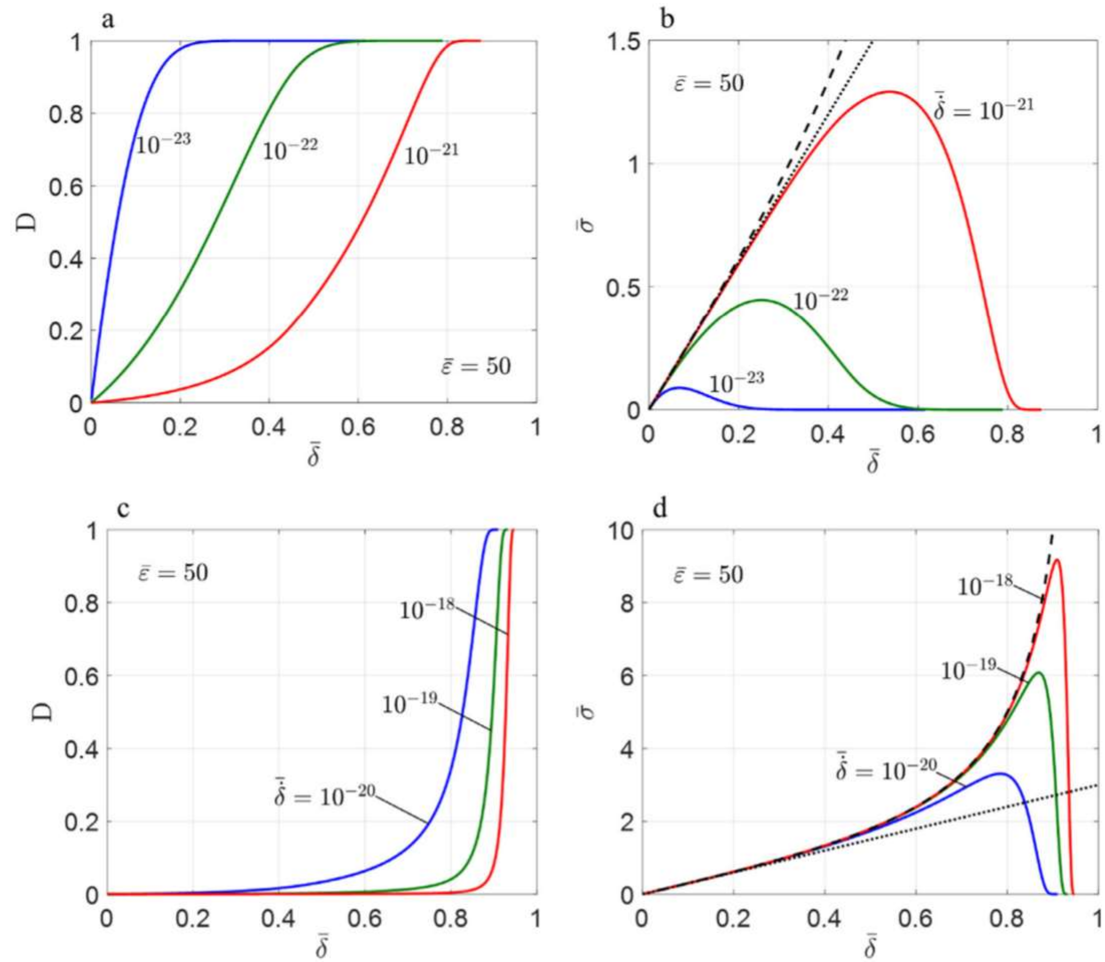
$$\bar{\dot{\delta}} = \frac{\dot{\delta} t_0}{n^2 r_0}$$

$$\bar{\varepsilon} = \frac{\varepsilon_0}{k_B T}$$

$$\sigma = (1 - D) N_0 f(\delta)$$

$$\frac{dD}{dt} = \frac{n}{t_0}(1 - D)\exp\left(-\frac{E_b}{k_B T}\right)$$

$$E_b \approx \varepsilon_0\left(1 - 1.664\hat{f}^{6/7} + \hat{f} + 0.0236\hat{f}^2\right)$$



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Rate-dependent interfacial properties

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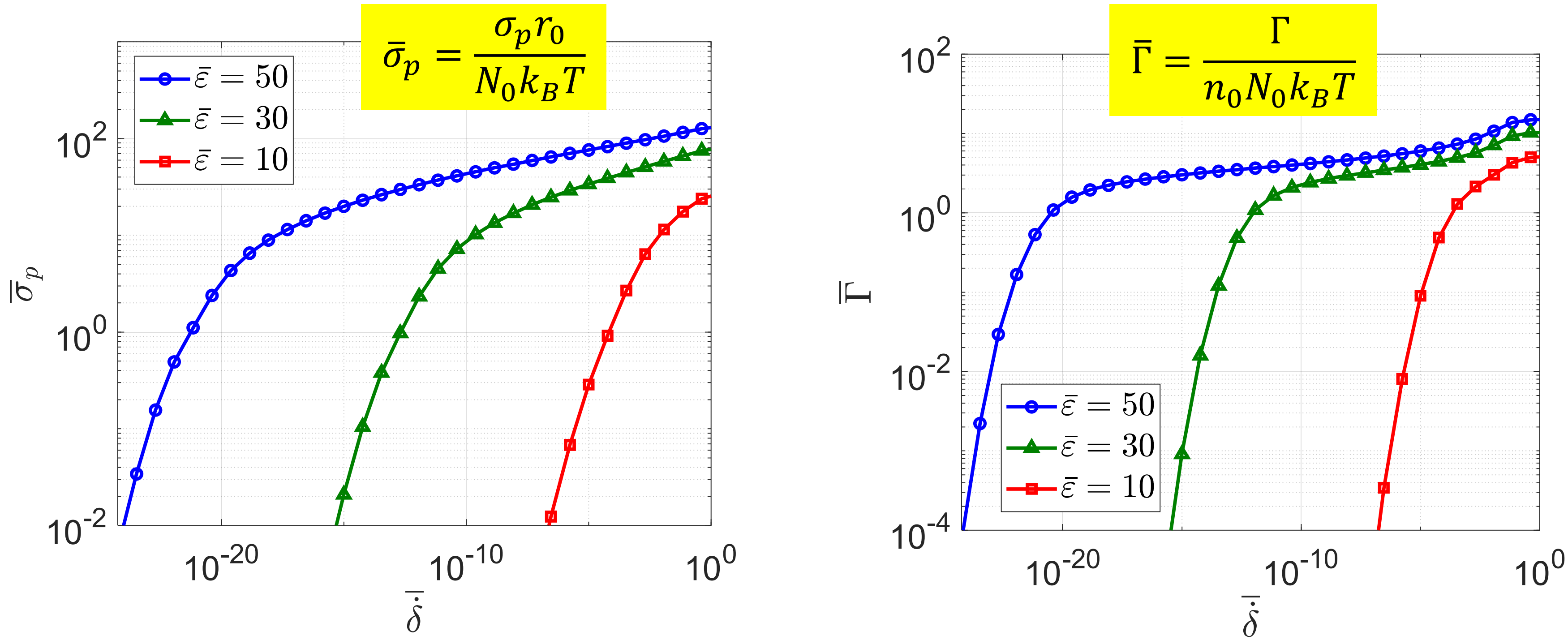

- The initial stiffness is *independent* of the separation rate.
- Both strength and toughness increase with increasing rates.
- The predicted toughness is always less than that by the Lake-Thomas model ($\bar{\Gamma} = \bar{\varepsilon}$).

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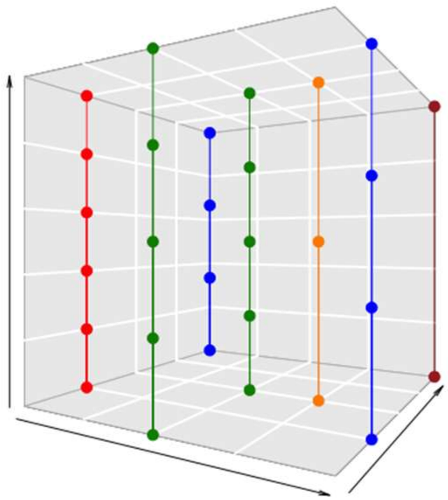
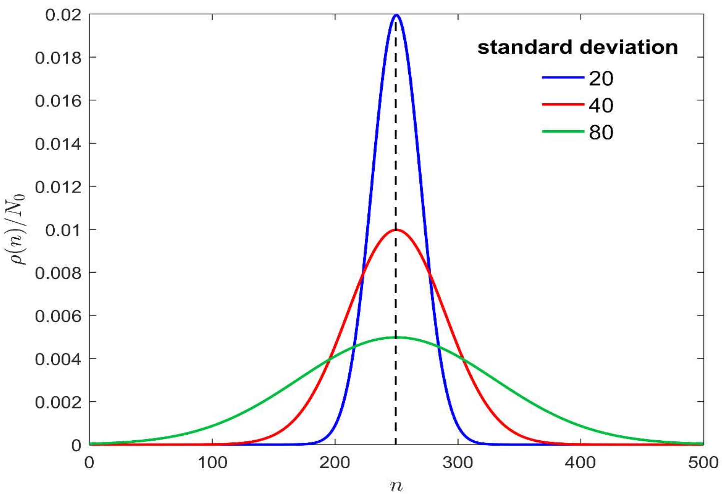
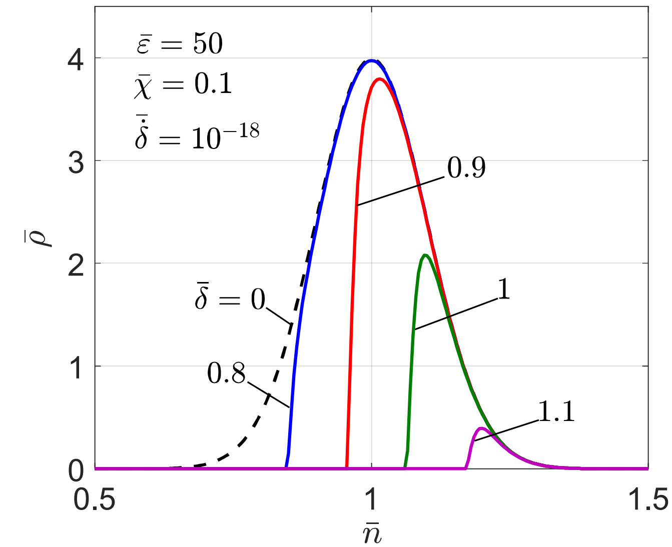
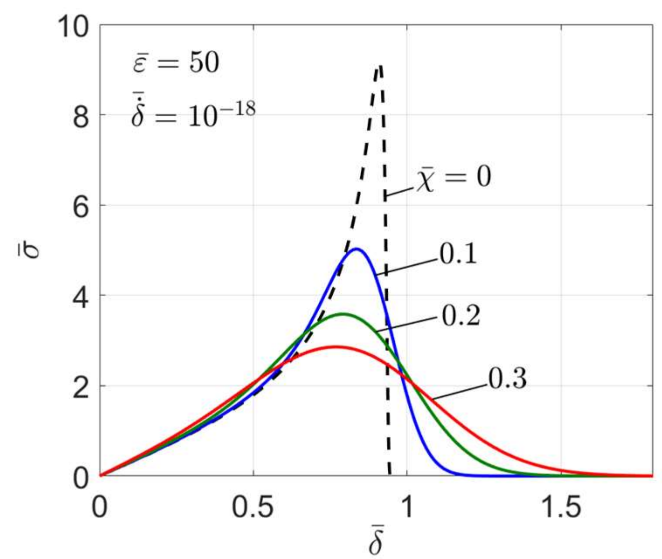
Effect of statistically distributed chain lengths





$$\rho_0(n) = \frac{N_0}{\sqrt{2\pi}\chi} \exp\left(-\frac{1}{2}\left(\frac{n-n_0}{\chi}\right)^2\right)$$





$$\lambda_n = \delta/(nr_0)$$

$$\sigma = \int (1 - D_n) f(\lambda_n) \rho_0(n) dn$$

$$\frac{dD_n}{dt} = \frac{n}{t_0}(1 - D_n)\exp\left(-\frac{E_b}{k_B T}\right)$$

The shorter chains break earlier, leading to lower strength. The presence of longer chains extends the range of separation.

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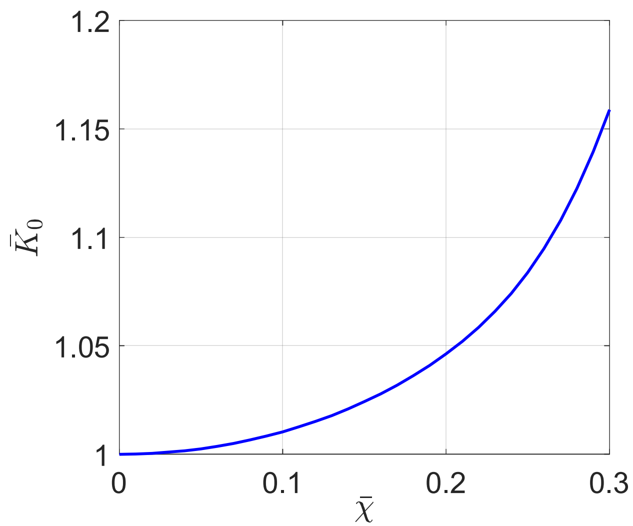
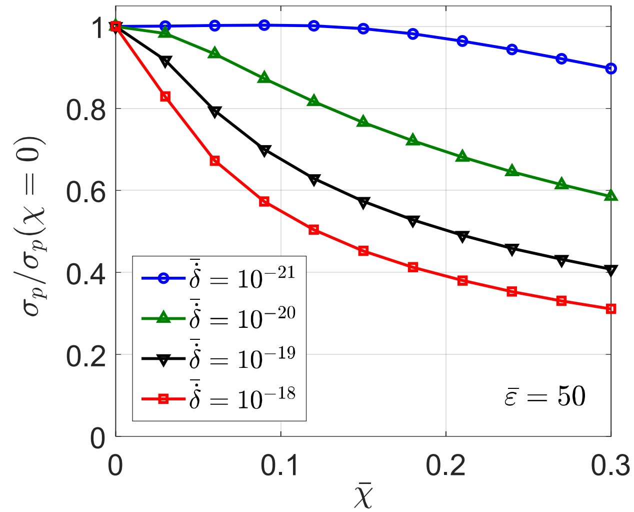
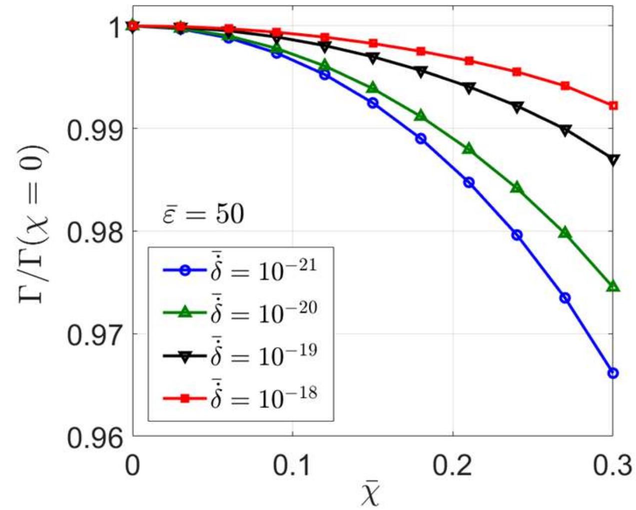
Effect of chain length distribution on interfacial properties

$$\bar{\chi} = \frac{\chi}{n_0}$$







- Interfacial stiffness: increases slightly, independent of rate
- Interfacial strength: decreases significantly with the relative deviation at fast rate
- Interfacial toughness: less sensitive to the chain length distribution

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Finite element implementation (ABAQUS/UINTER)

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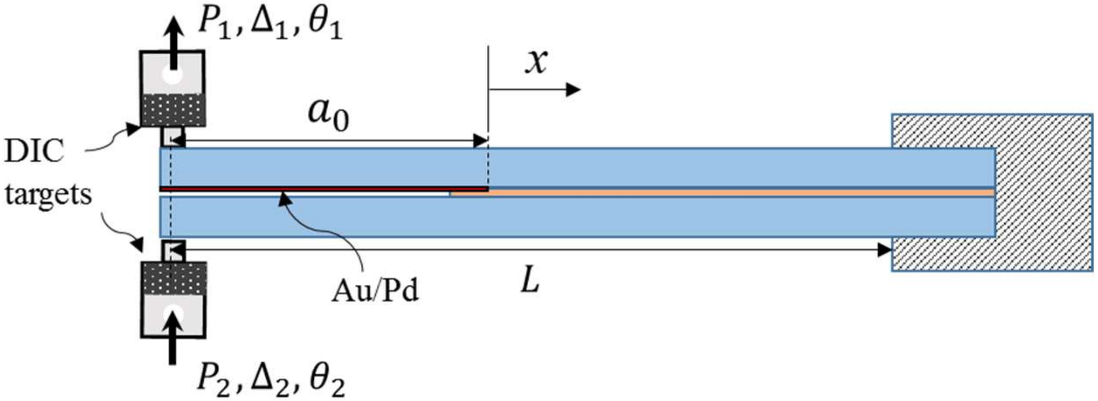
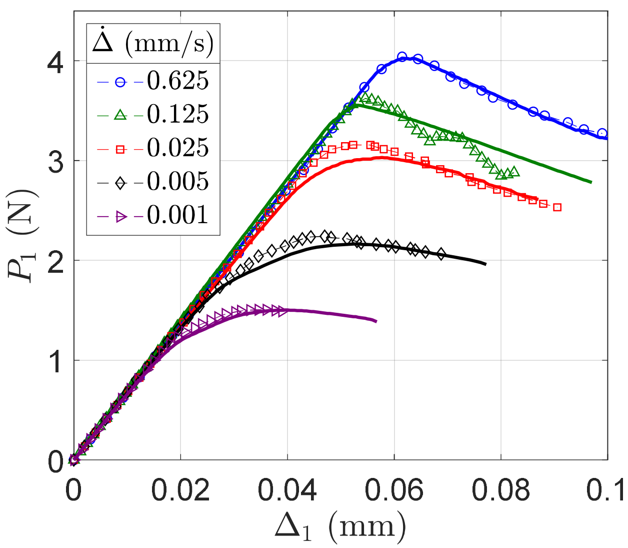
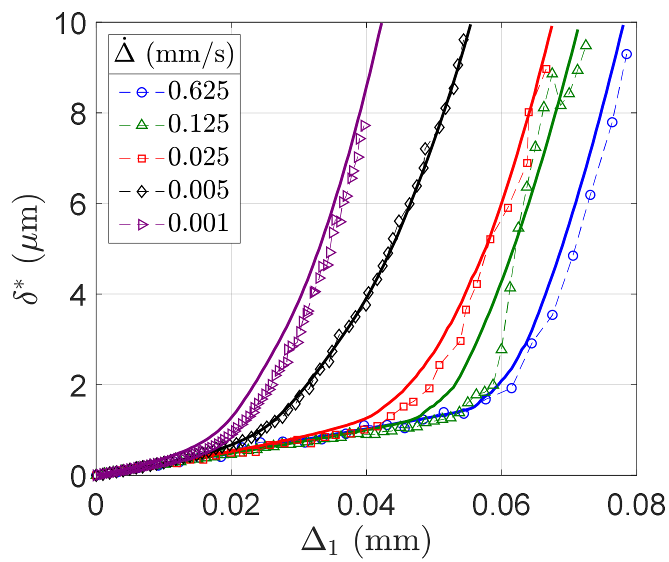
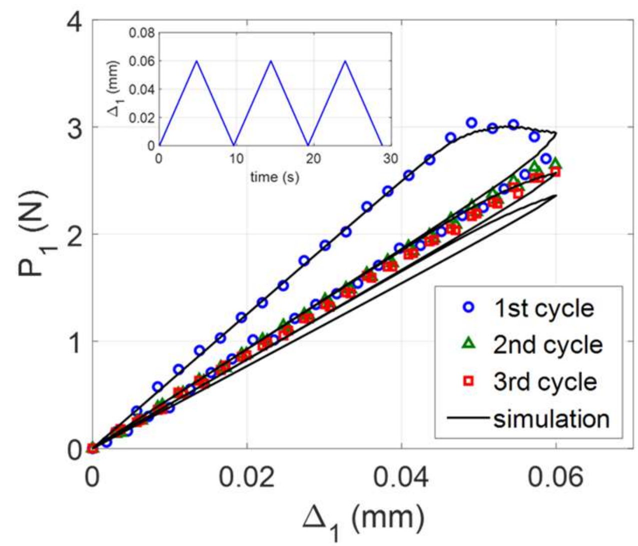


Model parameters:

- Bond length ($r_0 \sim 0.5$ nm)
- Bond energy ($\varepsilon_0 \sim 1$ eV)
- Average chain length ($n_0 \sim 4000$)
- Chain length deviation ($\chi \sim 230$)
- Chain areal density ($N_0 \sim 8 \times 10^{17}$ m^{-2})
- Microscopic time scale ($t_0 \sim 10^{-13}$ s)

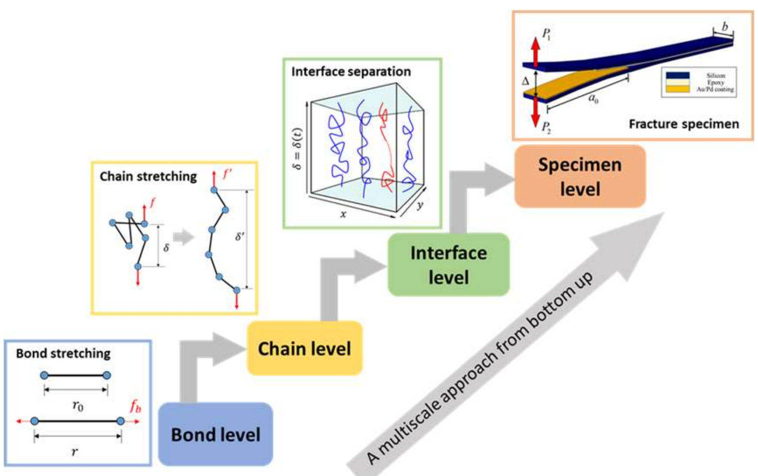


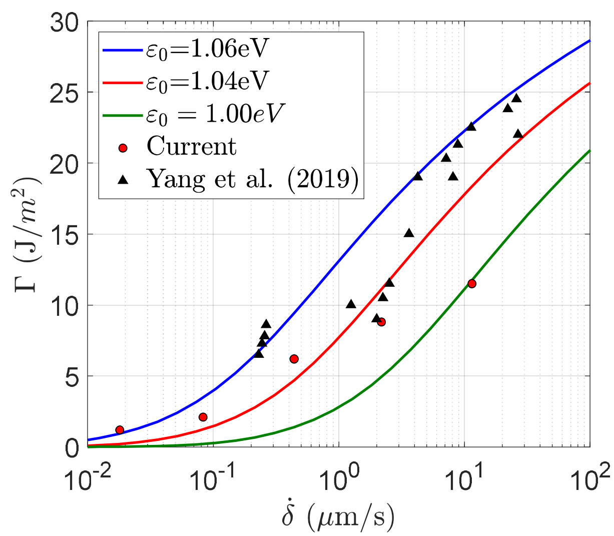


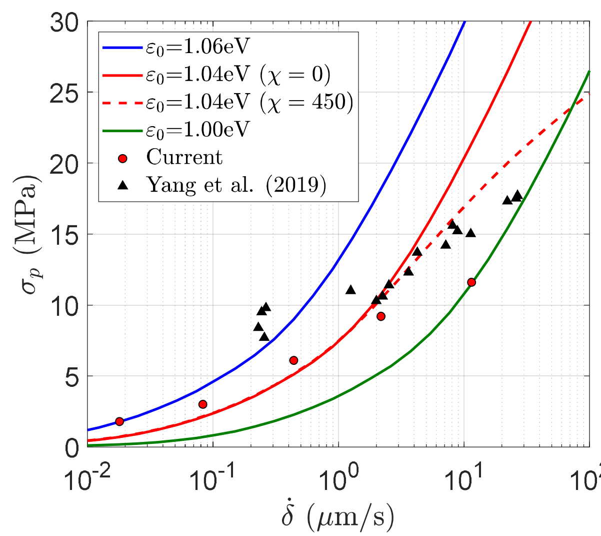


Summary

- A multiscale, mechanism-based cohesive zone model was proposed for rate-dependent fracture of polymer interfaces, potentially linking the interfacial properties (i.e., stiffness, strength and toughness) to the molecular structures.
- Model parameters were determined by direct comparation to the DCB experiments.
- The predicted traction-separation relation depends on the *local* separation rate and the loading history (e.g., non-monotonic or cyclic).







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