Fracture Behavior of API-60 DDS Epoxy Using MD Simulation

Chang Woon Jang
KBR Wyle
Intelligent Systems Division, NASA Ames Research Center

Wayne J. Mullinax
KBR Wyle
Intelligent Systems Division, NASA Ames Research Center

John W. Lawson
Intelligent Systems Division, NASA Ames Research Center

TABLE OF CONTENTS

01. Background of the study

Classical MD epoxy model and elastic property prediction

02. Method Development

Bond breaking Morse potentials from *ab intio* calculation

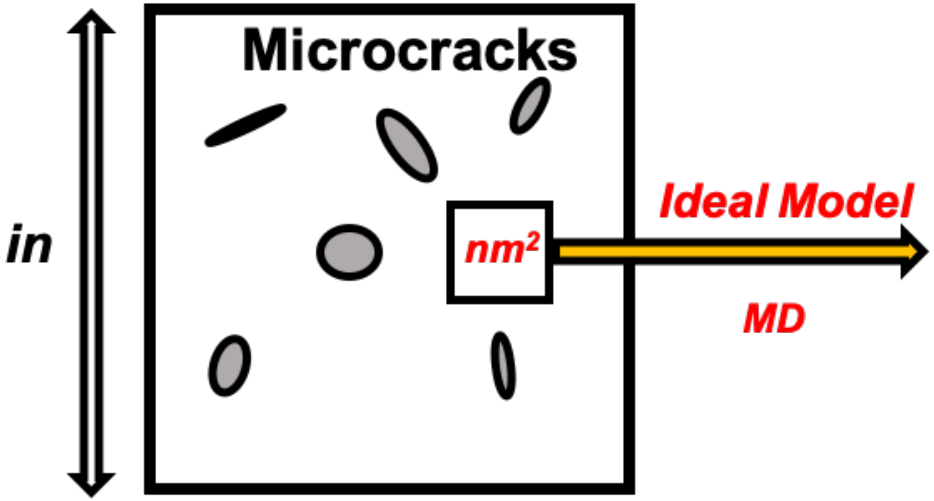
03. Results

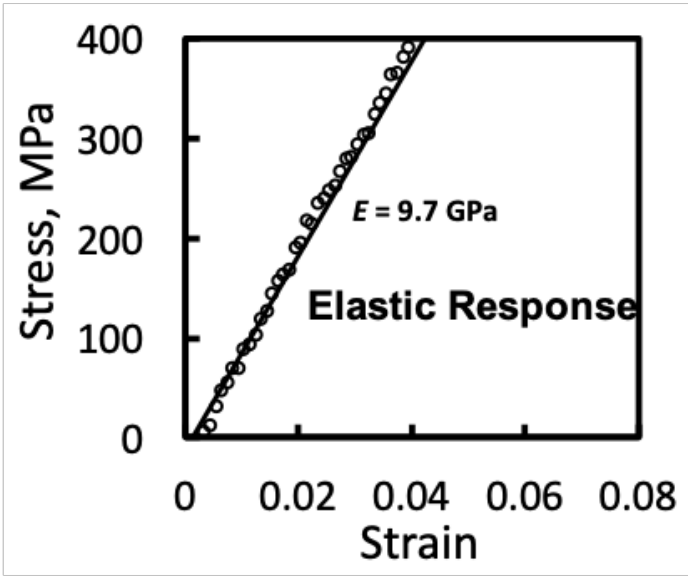
I) Tensile simulations and stress-strain behavior comparison: GAFF and Morse

II) Key mechanism of epoxy brittle behavior with crack inclusion

04. Summary and Conclusion

Background of the Study





- Classical epoxy MD models contain ***no defects***
- Only allow for ***elastic property prediction and no Fracture***
- ***Very high mechanical property***

Fracture Model Structures

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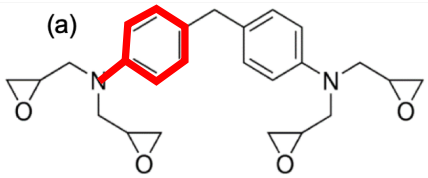
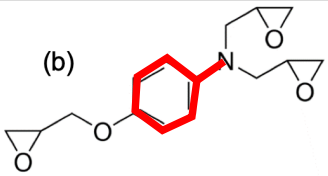
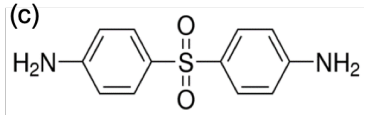
Tetra-functional Epoxy



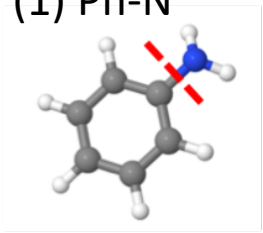
Tri-functional Epoxy



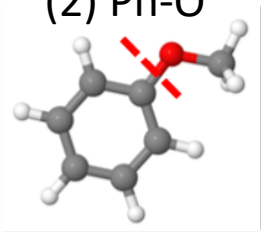
Hardener



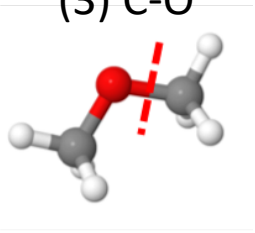
(1) Ph-N



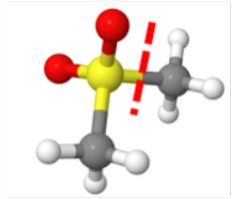
(2) Ph-O



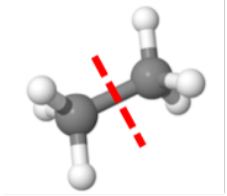
(3) C-O



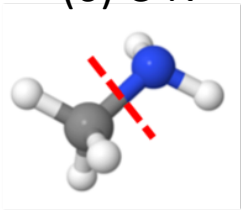
(4) C-S



(5) C-C



(6) C-N



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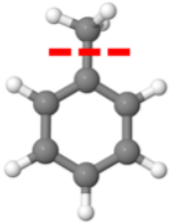

All backbone bonds

Computational Chemistry for Bond Breaking

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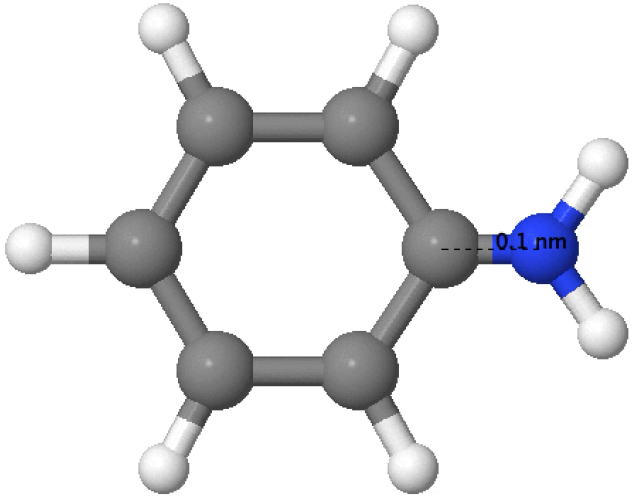
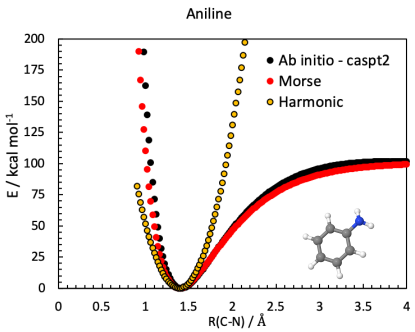
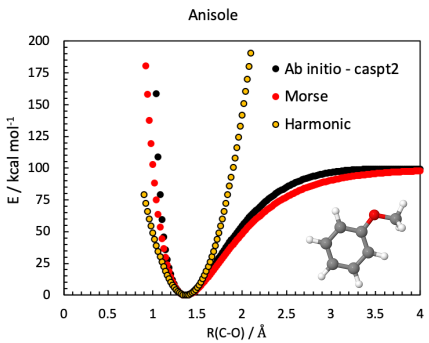
Animation

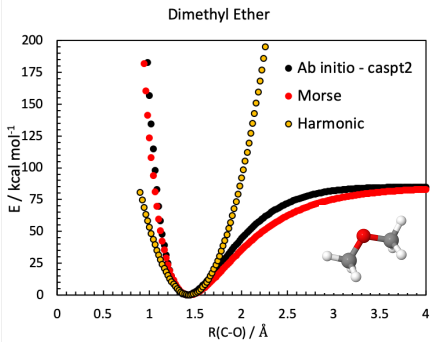


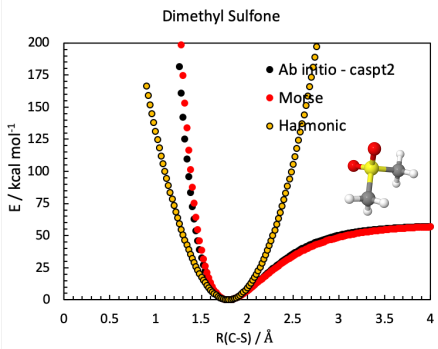
High accuracy computational chemistry simulation

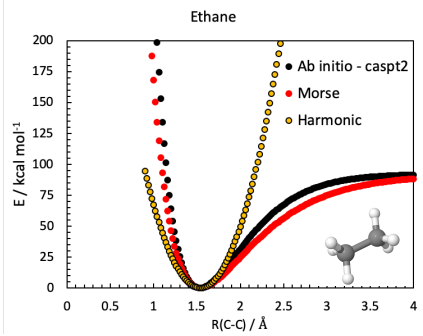
Comparison of Morse and GAFF Bond FF

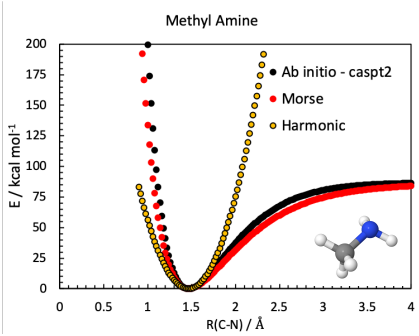


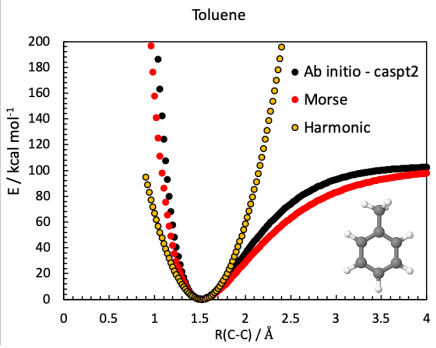












Morse Bond Potential $V(r) = D_e\left(1 - e^{-\alpha(r-r_e)}\right)^2$

Hybrid Potential Functions with Bond Breaking

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$$V(r) = D_e\left(1 - e^{-\alpha(r-r_e)}\right)^2 + \sum_b k_b(b-b_0)^2 + \sum_\theta k_\theta(\theta-\theta_0)^2 + \cdots$$

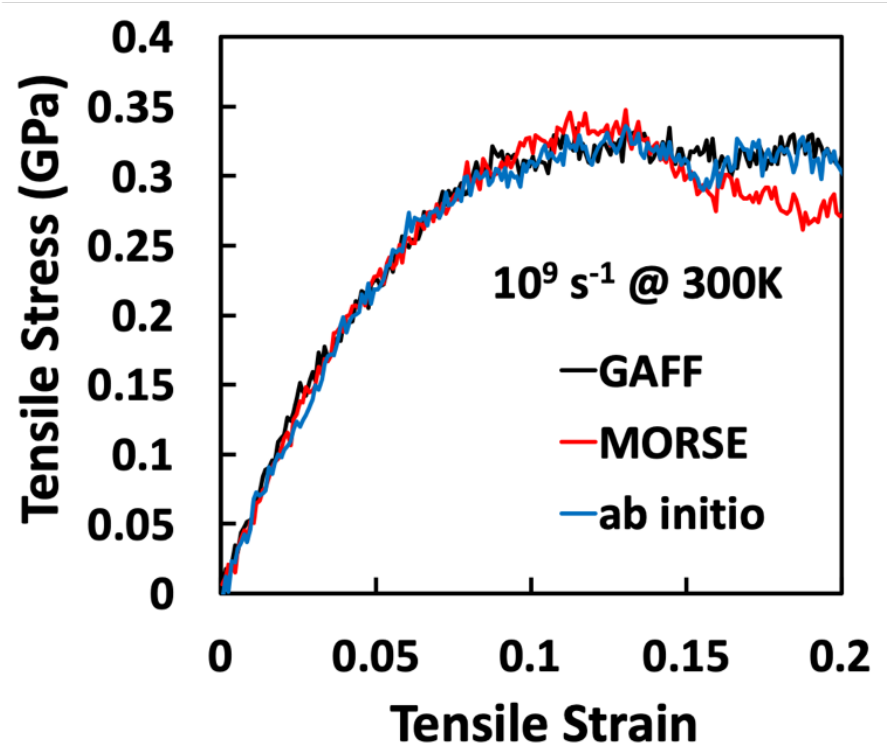
Morse Bond — GAFF

$$\cdots + \sum_d \frac{k_\varphi}{2}[1+\cos(n\varphi-\gamma)] + \sum_{i<j}\left[\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}} + C\frac{q_i q_j}{r_{ij}}\right]$$

GAFF

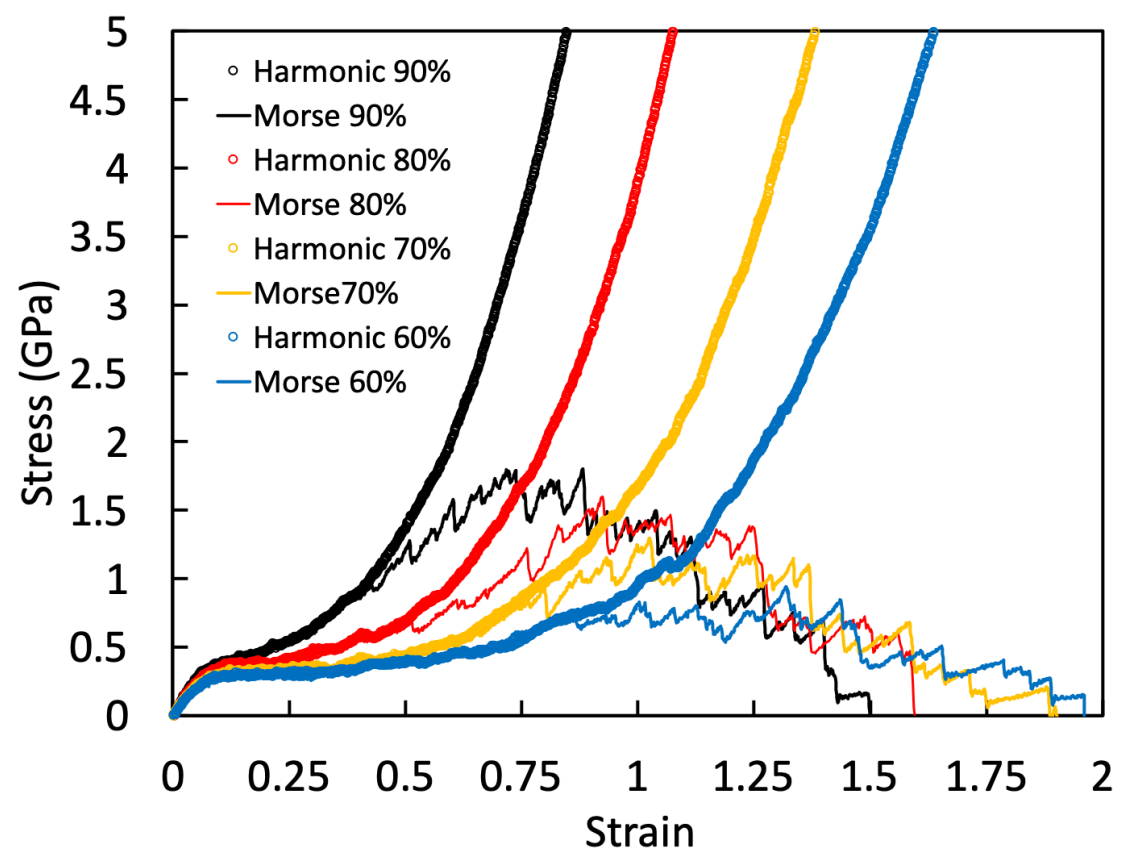
- GAFF: a majority of interactions, Morse: breaking bonds of backbone
- Maintain computational efficiency – Minimal change of potential functions
- GAFF: 1 fs time step >> ReaxFF: 0.1 fs time step

Tensile Simulations with Hybrid Potential



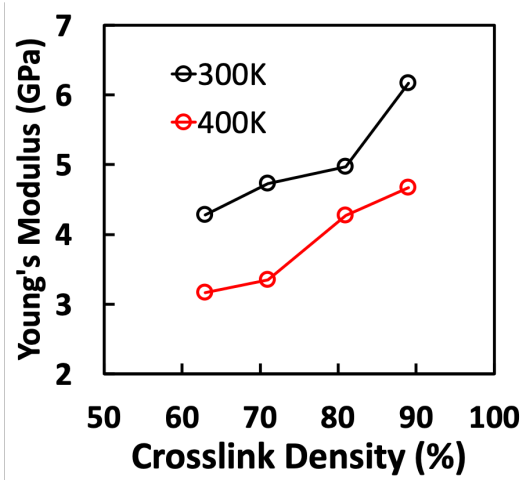
Verify correct elastic behavior with new potential function

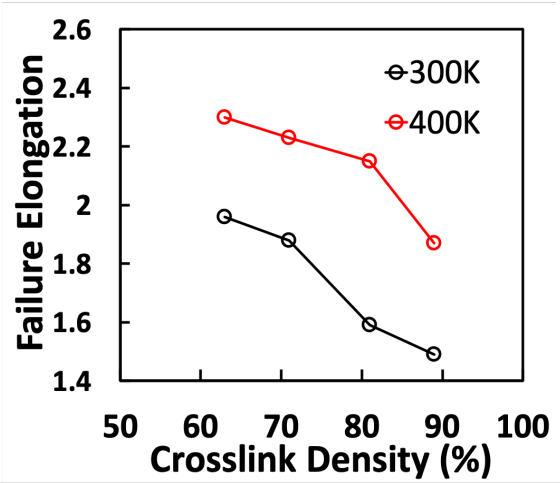
Stress-Strain Curves : Harmonic vs Morse

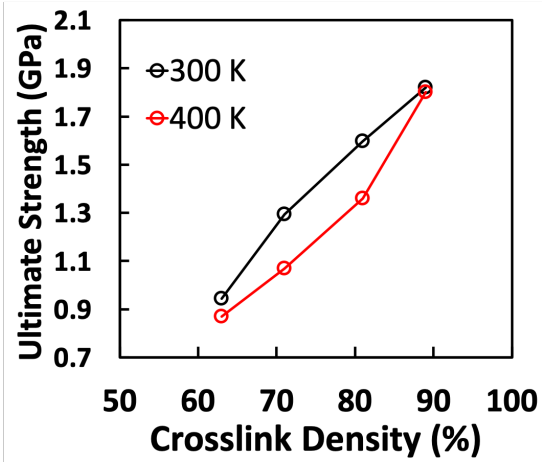


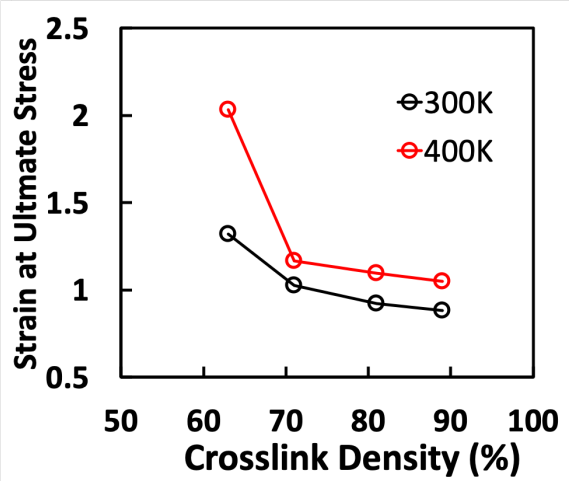
- Both potentials have similar elastic behavior
- Morse potential describes material failure at higher strains

Elastic and Inelastic Mechanical Properties

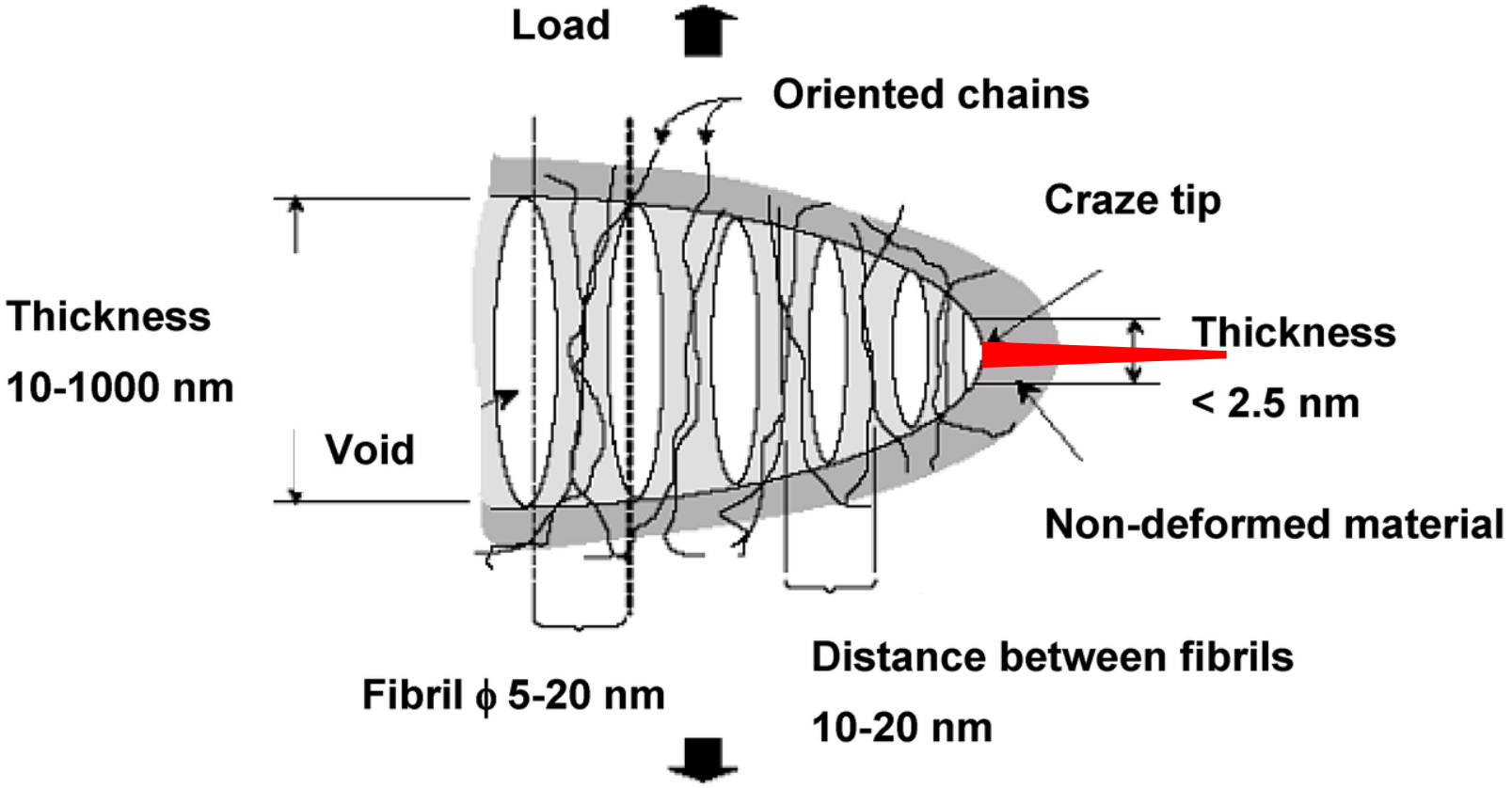








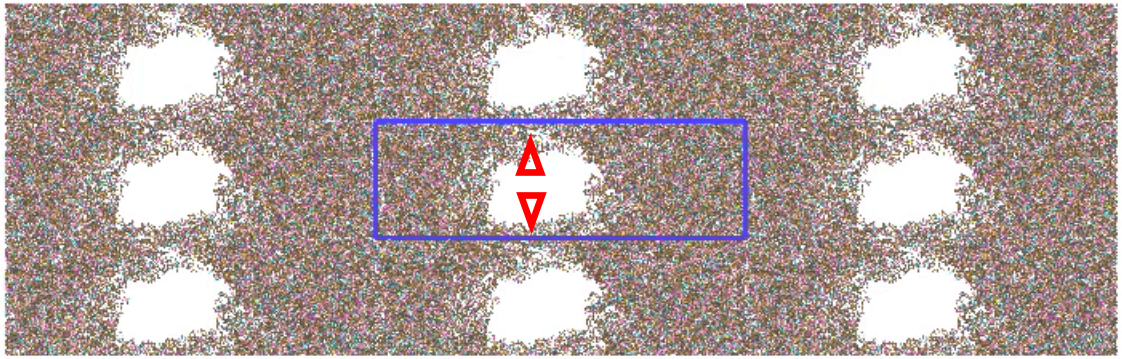
Crack Formation and Failure Mechanism



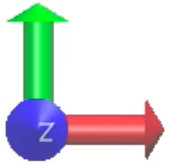
Want to include these mechanism in simulations

Simulations Including Defects

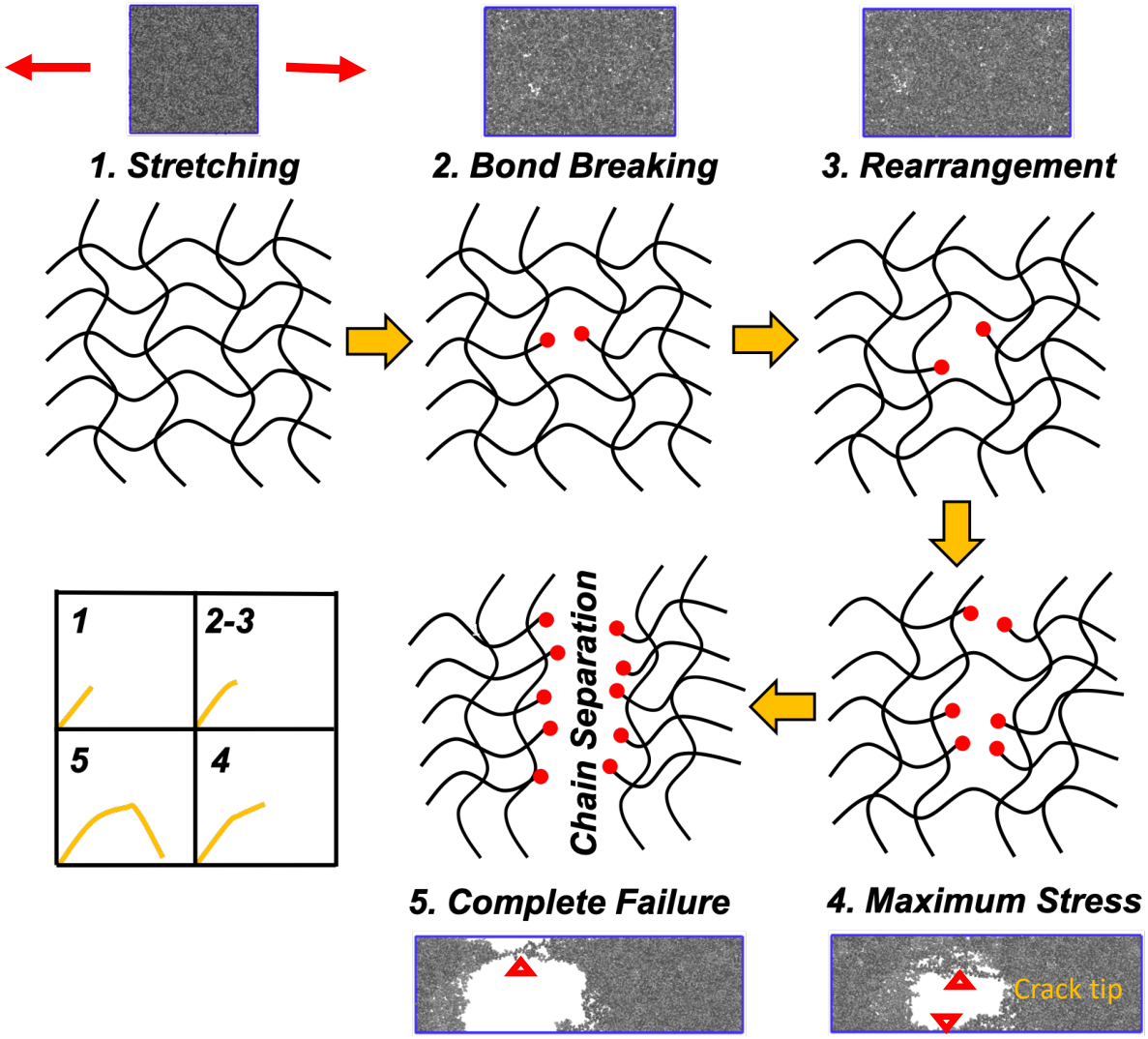
Failure Direction



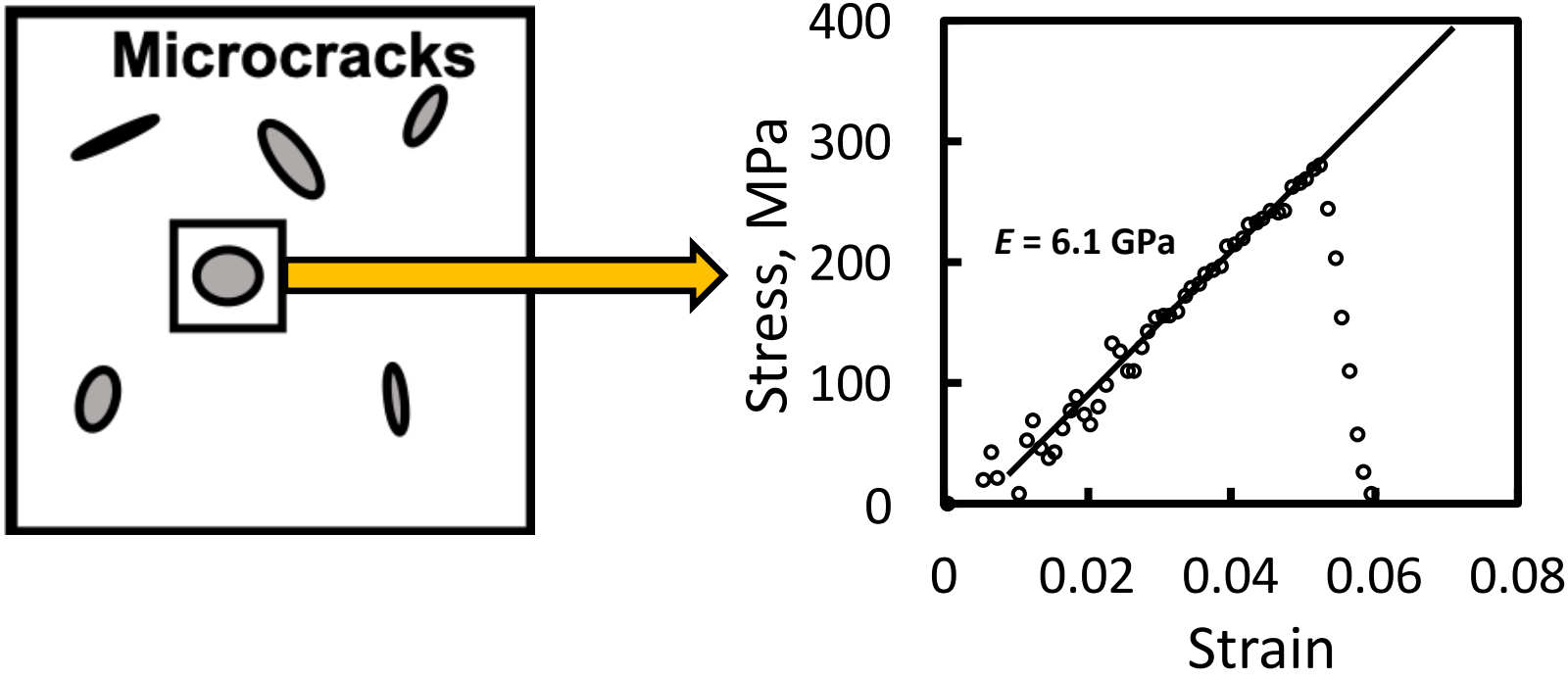
Tensile Direction



Failure Mechanisms from Simulations

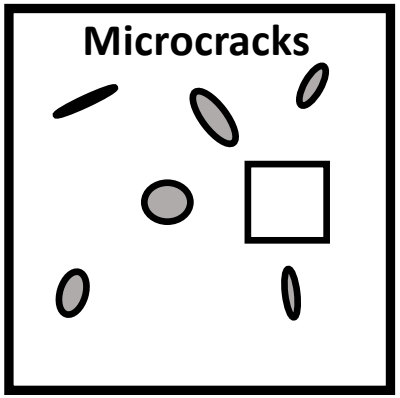


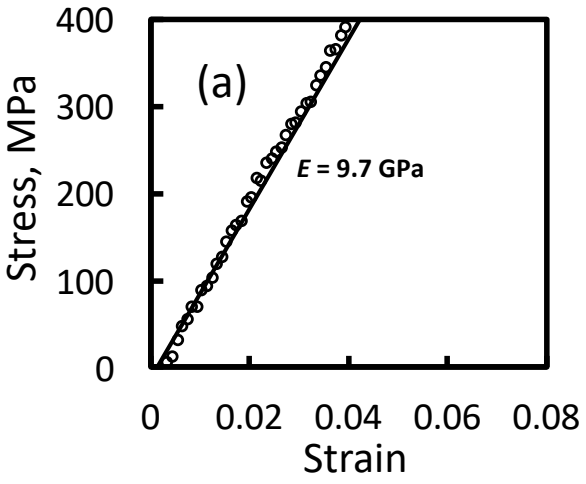
Stress-Strain Curve with Microcracks



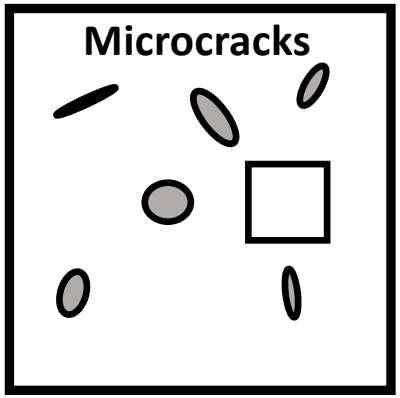
Brittle Epoxy Failure

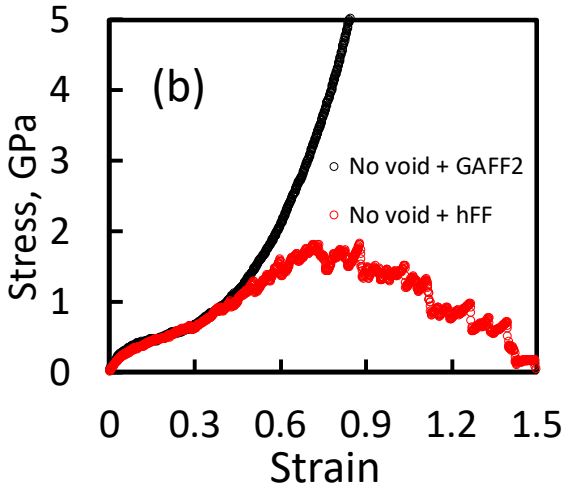
Summary



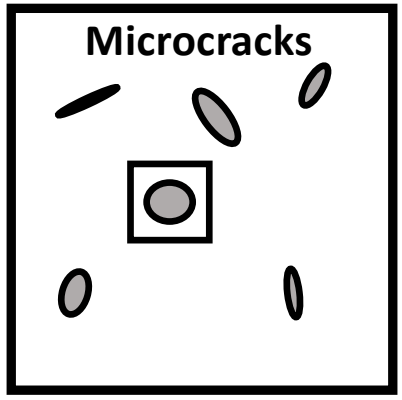


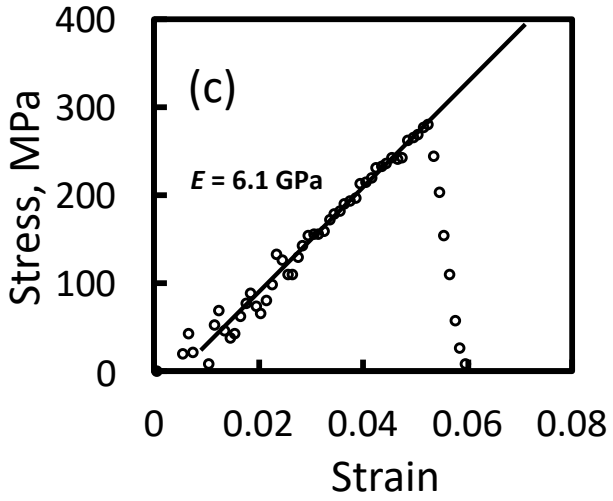
- *Good elastic behavior*
- *No Failure*





- *Good elastic behavior*
- *Failure included*

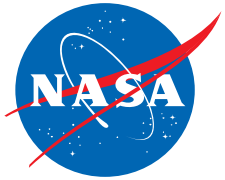




- *Improved elastic prediction*
- *Improved failure prediction*

Conclusion

- Hybrid force field (***GAFF + Morse***) was developed to investigate ***elastic and plastic behavior*** of an epoxy system using MD simulations
- Hybrid force field reproduced ***the elastic behavior*** from GAFF
- We captured ***bond breaking*** and ***failure behavior***
- The existence of crack can determine ***the brittle behavior*** of epoxy system
- Development of ***an-harmonic angle and dihedral potentials*** would allow for predicting ***more accurate plastic behavior*** of the crosslinked epoxy



Acknowledgement

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