Degradation of Carbon Fiber Microstructures due to Oxidative Etch Pitting

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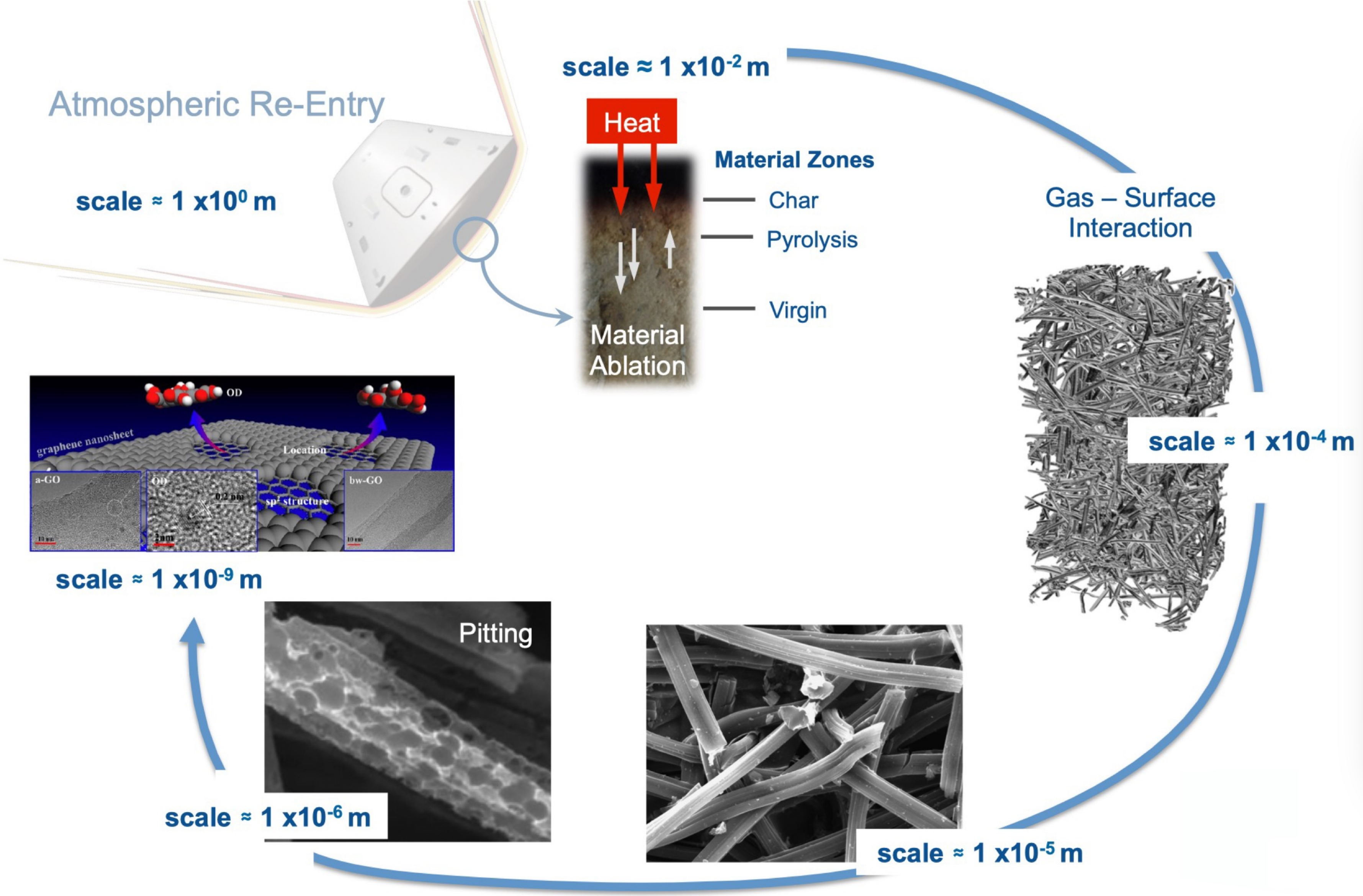
Motivation



Overall Objective:

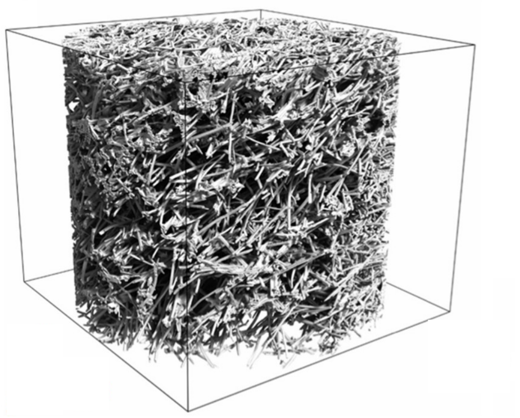
Characterize/predict effects of etch pitting on performance/failure of carbon ablators

Current Objective:

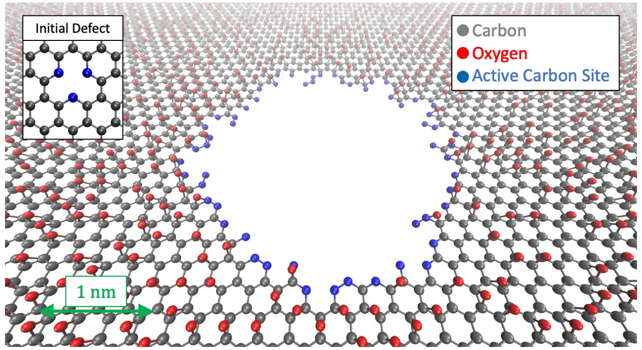
- Simulate pitting of carbon microstructures
- Analyze degradation of relevant material properties

Approach + Tools Overview

Inputs

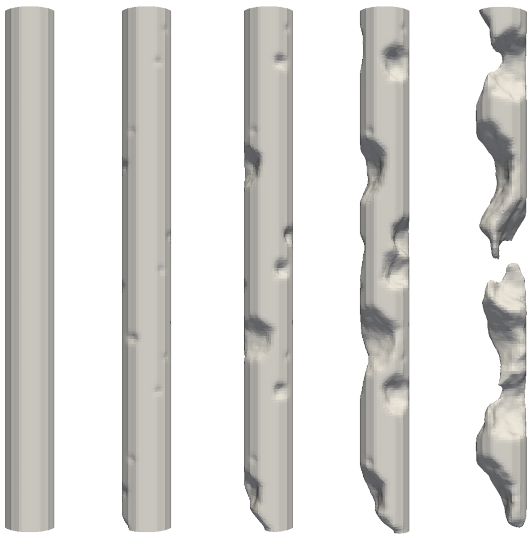


Microstructure (µCT)



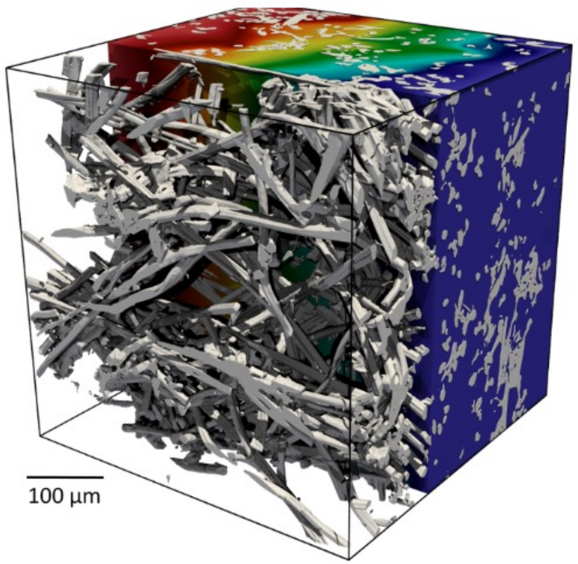
Surface Oxidation Model
+ Pitting Rates

Pitting Simulations



SPARTA (DSMC)
+ Active Sites

Material Property Calculations

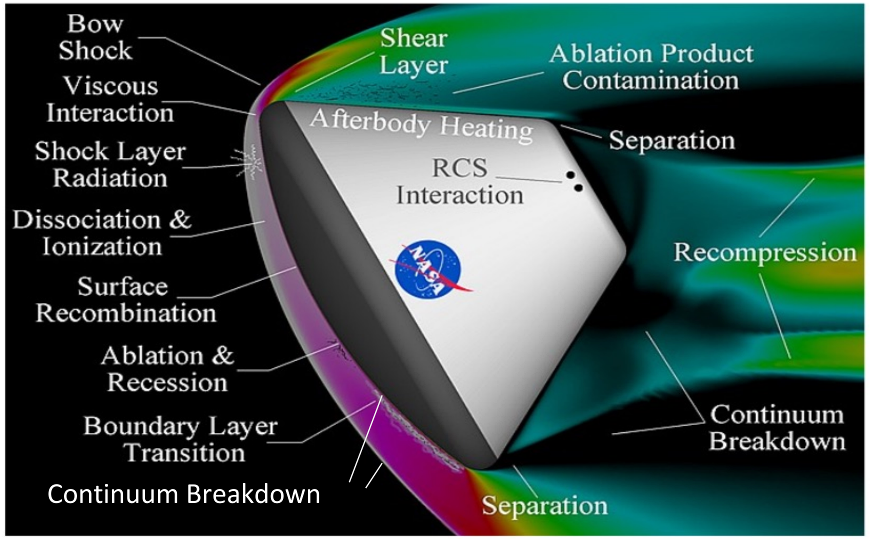


Porous Microstructure
Analysis (PuMA)

SPARTA + Active Site Implementation

Why DSMC?

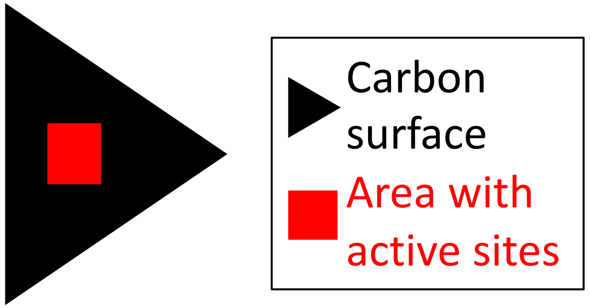
- Regions of continuum breakdown in reentry flow
- DSMC is valid in all regimes: continuum, rarefied and transition (however computational cost increases with density)
- DSMC (direct simulation Monte Carlo) is a stochastic, particle-based method to solve the Boltzmann equation



[1] Plimpton, S. J., S. G. Moore, A. Borner, A. K. Stagg, T. P. Koehler, J. R. Torczynski, and M. A. Gallis. "Direct simulation Monte Carlo on petaflop supercomputers and beyond." *Physics of Fluids* 31, no. 8 (2019): 086101.

SPARTA + Pitting

- Open source, developed at Sandia
- Key Features:
  - Parallel implementation → large domains/long times
  - Reads µCT based structures → study real structures
  - Ablate function for recessing solid surfaces → simulate etch pitting
  - Detailed surface collisions and chemistry → key to pitting implementation
- New Implementation:
  - Active Site Fraction (ASF) as new quantity of surface elements → enables local reactivity differences
  - Reaction rate for CO formation linked to pitting rate



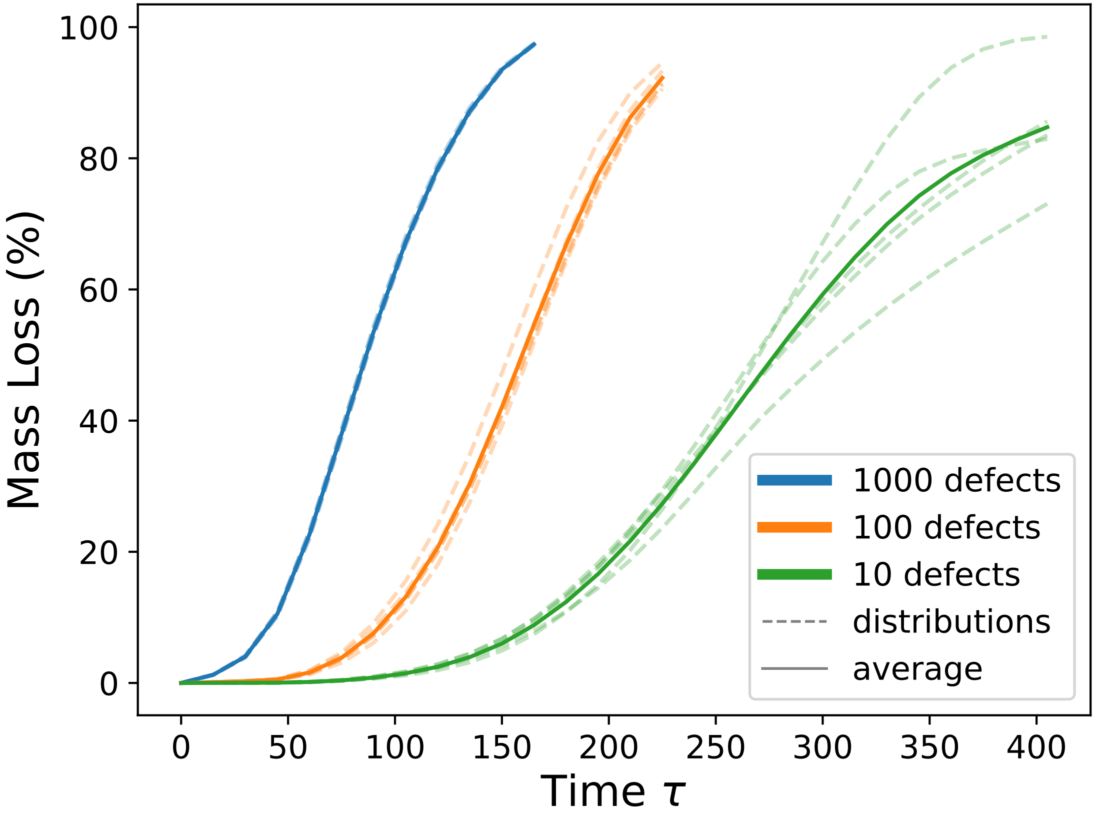
Pitting Simulation Results – Single Fiber

Simulation setup:

- Cylindrical fiber, 10 µm diameter, 100 µm length
- 0.5 µm voxel size
- Constant oxygen pressure
- Varying number of defects and distributions

Sample Simulation Video

Ablation rate dependency on defect density



→ More pits cause faster ablation

→ Variance with pit distribution is inversely related to number of pits

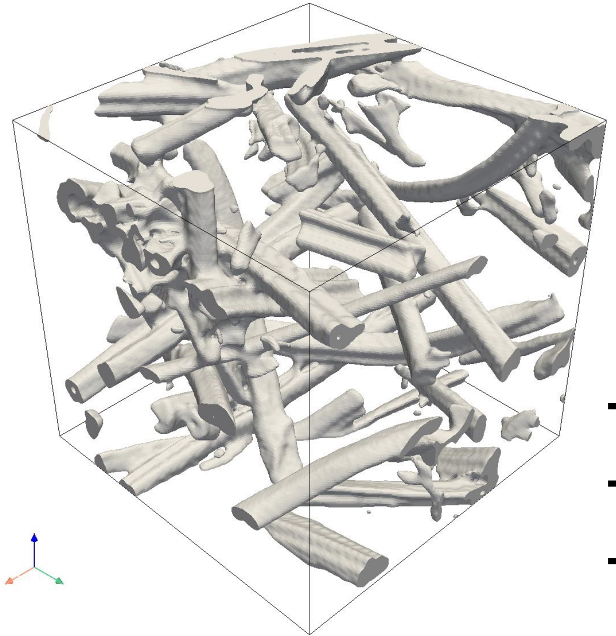
→ Pitting fragments fiber into chunks

Pitting Simulation Results – FiberForm

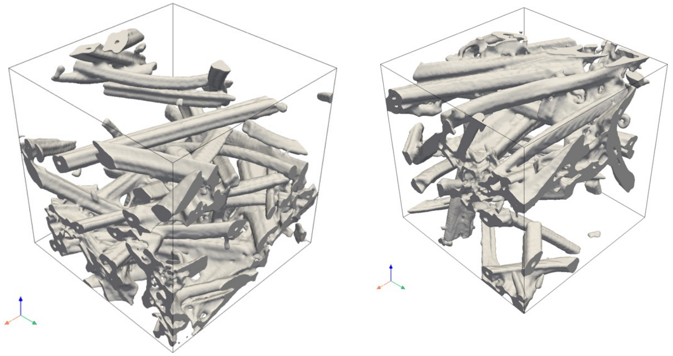
Simulation setup:

- Three 200^3 voxel substructures from FiberForm µCT scan
- 0.65 µm voxel size
- Constant oxygen pressure
- Varying number of defects and distributions

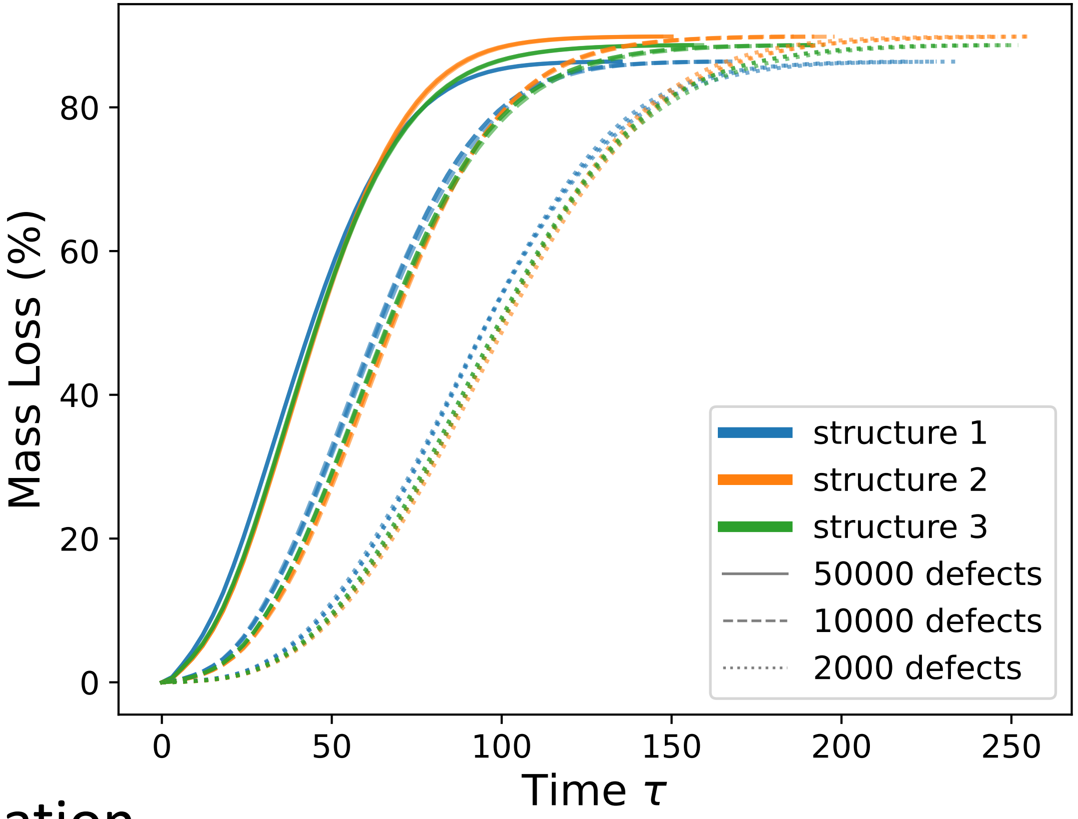
Sample Simulation Video



Other Substructures



Ablation rate dependency on defect density



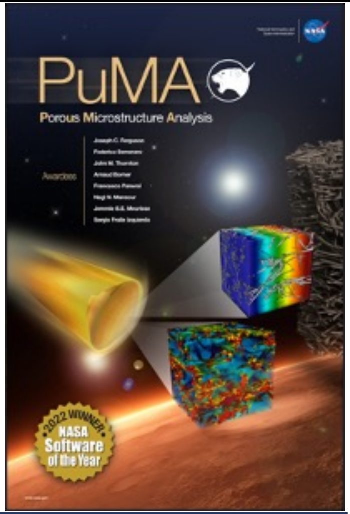
→ More pits cause faster ablation

→ Variance with pit distribution generally very low

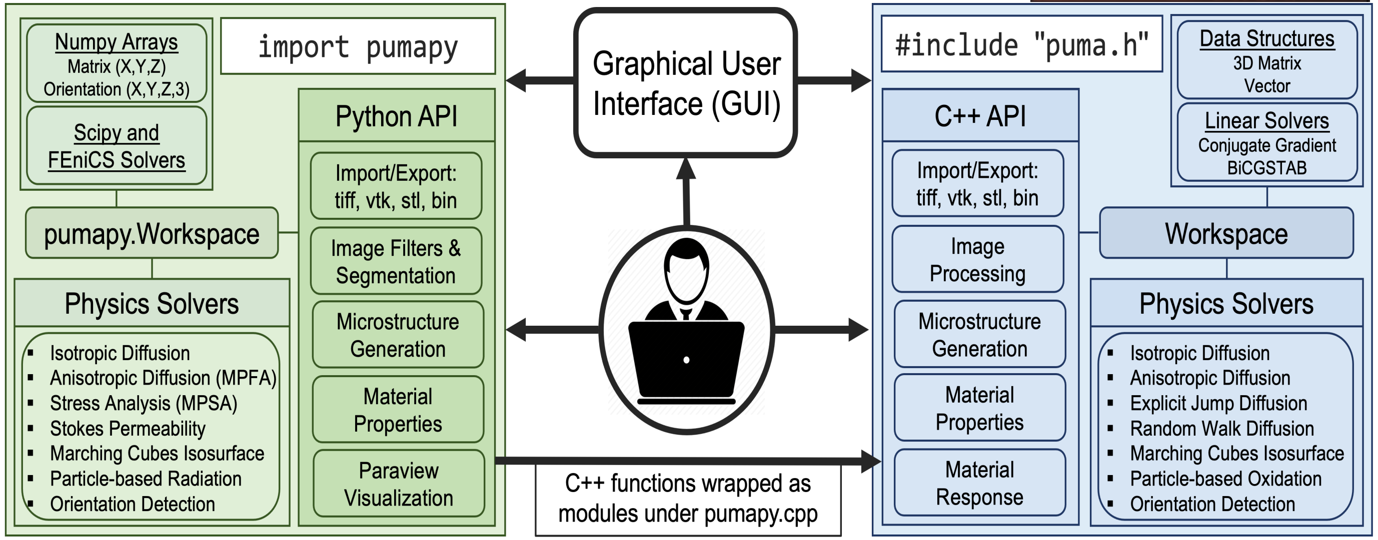
→ Variance between substructures

PuMA Overview

- Open source (https://github.com/nasa/puma)
- Developed at NASA Ames
- Installation: conda install -c conda-forge puma
- Software of the year



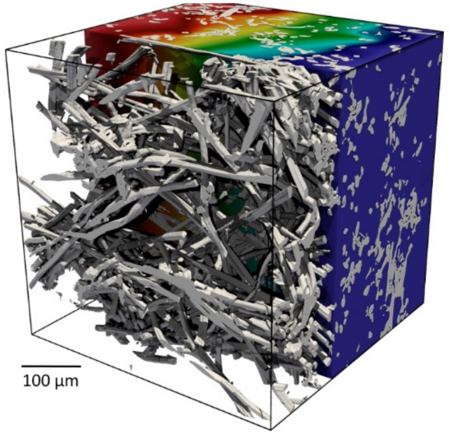
PuMA Architecture



[2] Ferguson, J.C., Semeraro, F., Thornton, J.M., Panerai, F., Borner, A. and Mansour, N.N., 2021. Update 3.0 to "PuMA: The porous microstructure analysis software". *SoftwareX*

Property Calculations

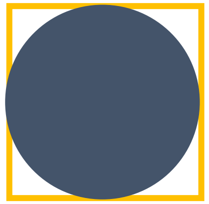
- Run simulation in each principal direction, imposing known displacement on each face, while keeping opposite face fixed (similar for temperature gradient)
- Apply symmetry/periodic BC on other faces
- Solve stress/temperature field inside material and obtain anisotropic elasticity tensor C, or thermal conductivity tensor K
- Assuming isotropic/ orthotropic behavior, obtain effective Young's moduli



Thermal Conductivity Results – Single Fiber

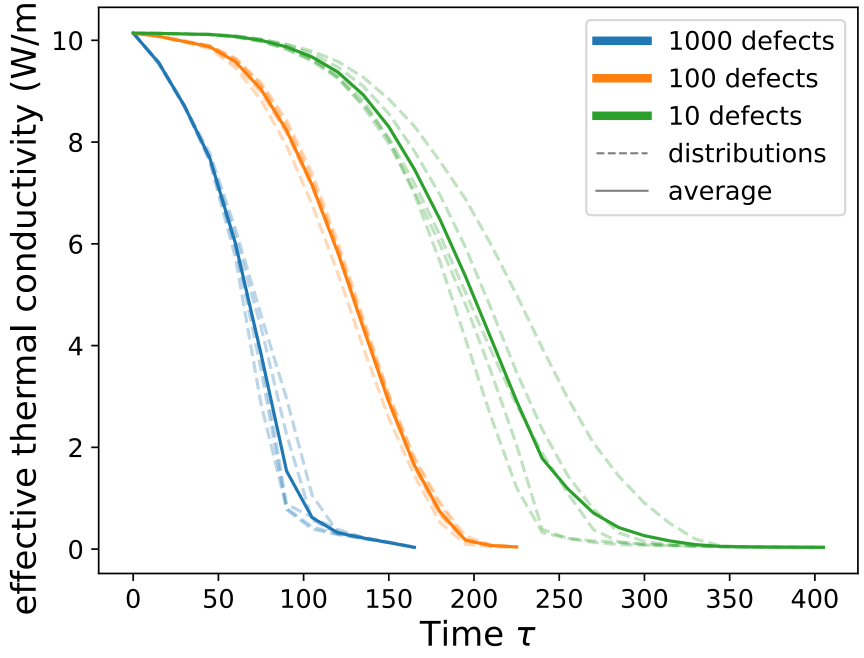
Intrinsic fiber properties

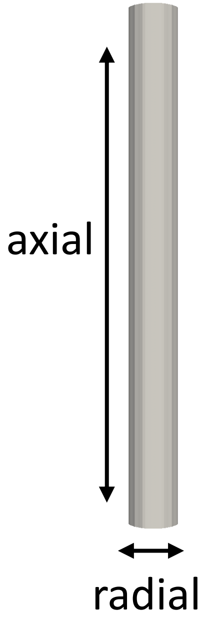
$$k_{axial} = 12\ \mathrm{W/mK}, k_{radial} = 0.7\ \mathrm{W/mK}$$



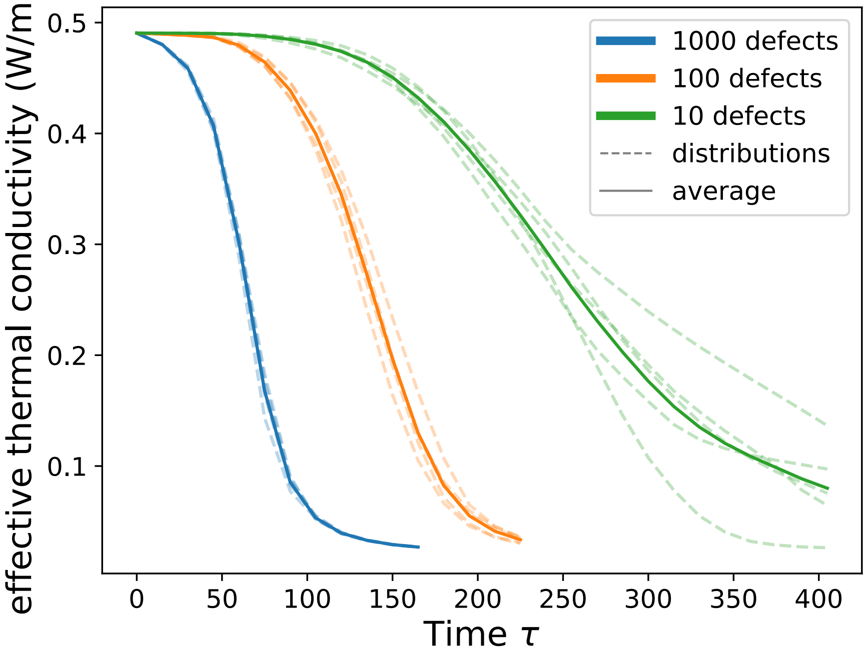
$$\frac{A_{circle}}{A_{square}} = \frac{4}{\pi} \approx 0.85 \text{ (due to segmentation)}$$

Axial Conductivity (in fiber axis)





Radial Conductivity (across fiber)

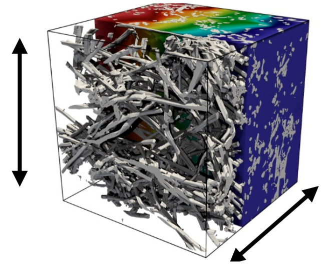


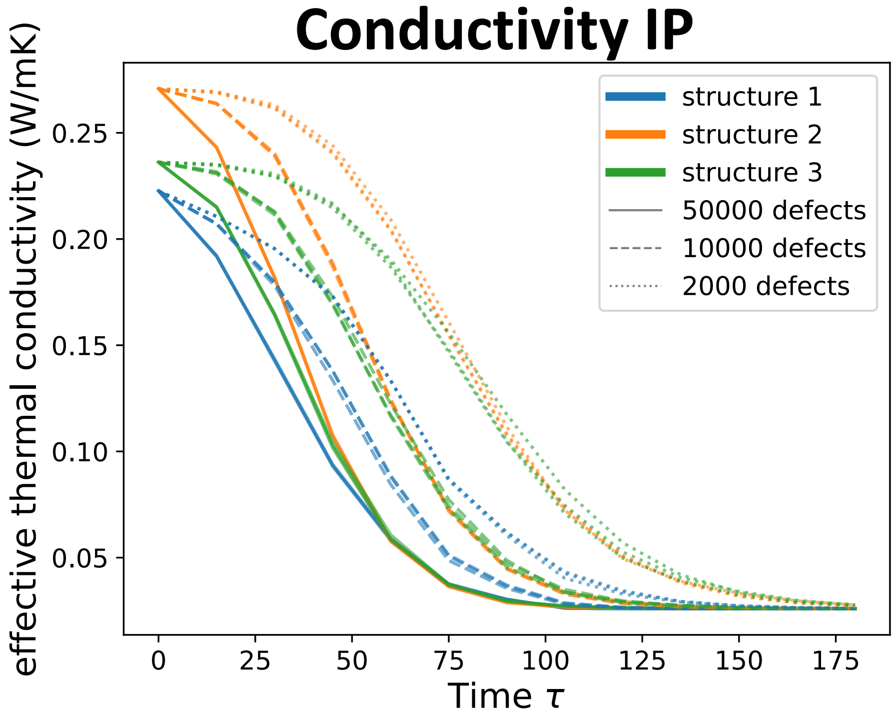
→ Thermal conductivity drops similarly in principle directions.

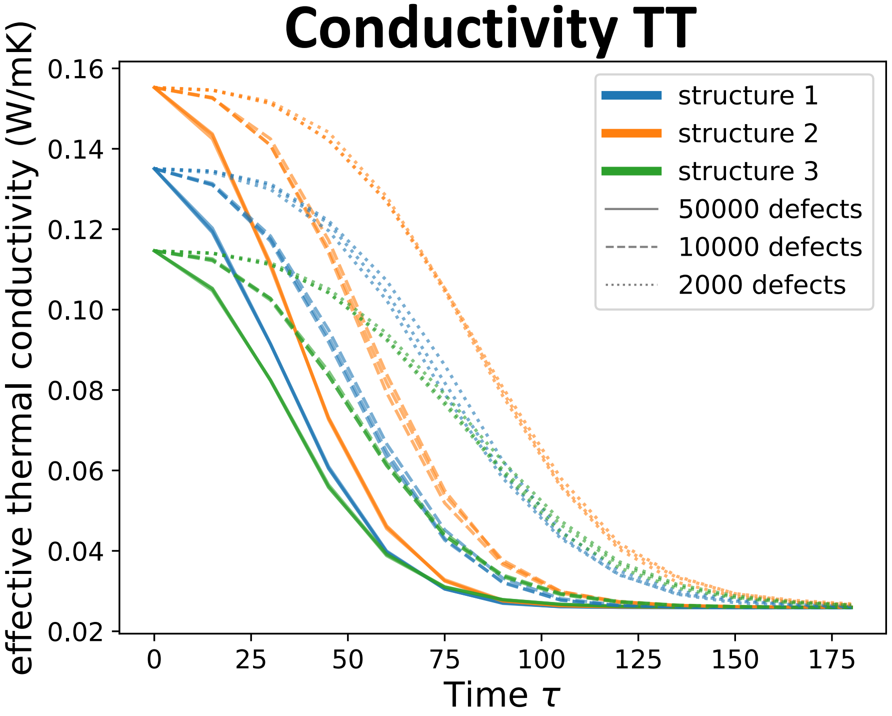
Thermal Conductivity Results – FiberForm

Intrinsic fiber properties

$$k_{axial} = 12 \text{ W/mK}, k_{radial} = 0.7 \text{ W/mK}$$







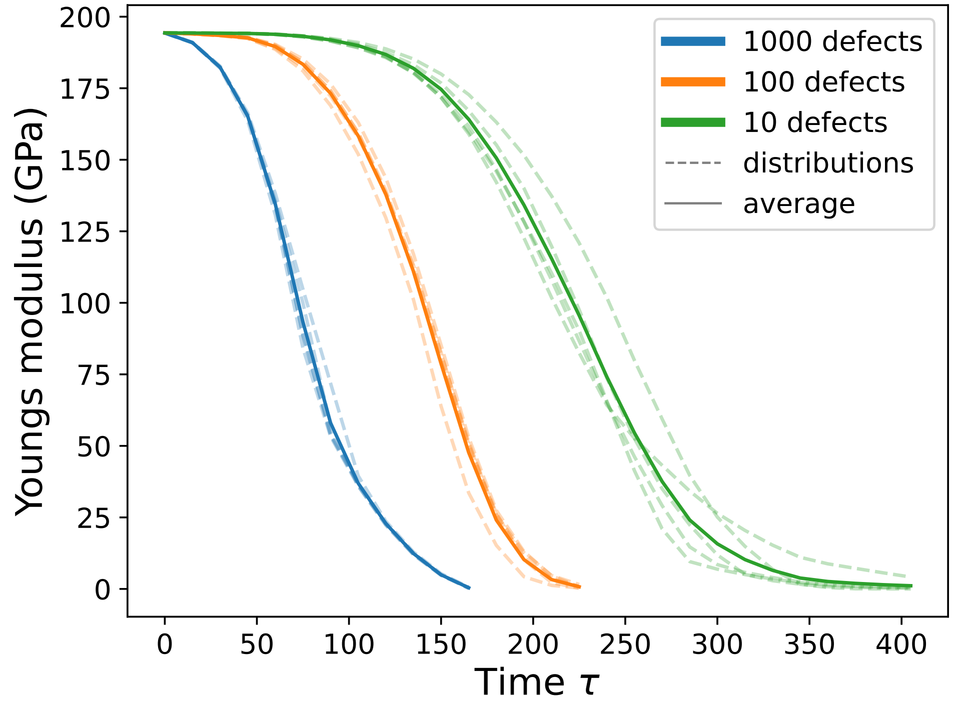
→ Influence of microstructure becomes apparent. This variance vanishes with larger sample sizes.

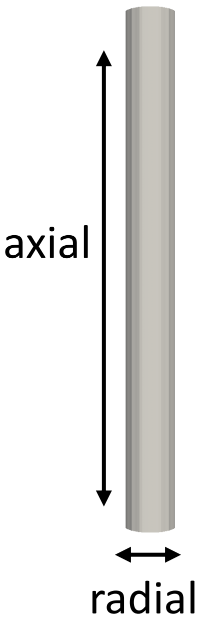
Linear Elasticity Results – Single Fiber

Intrinsic fiber properties

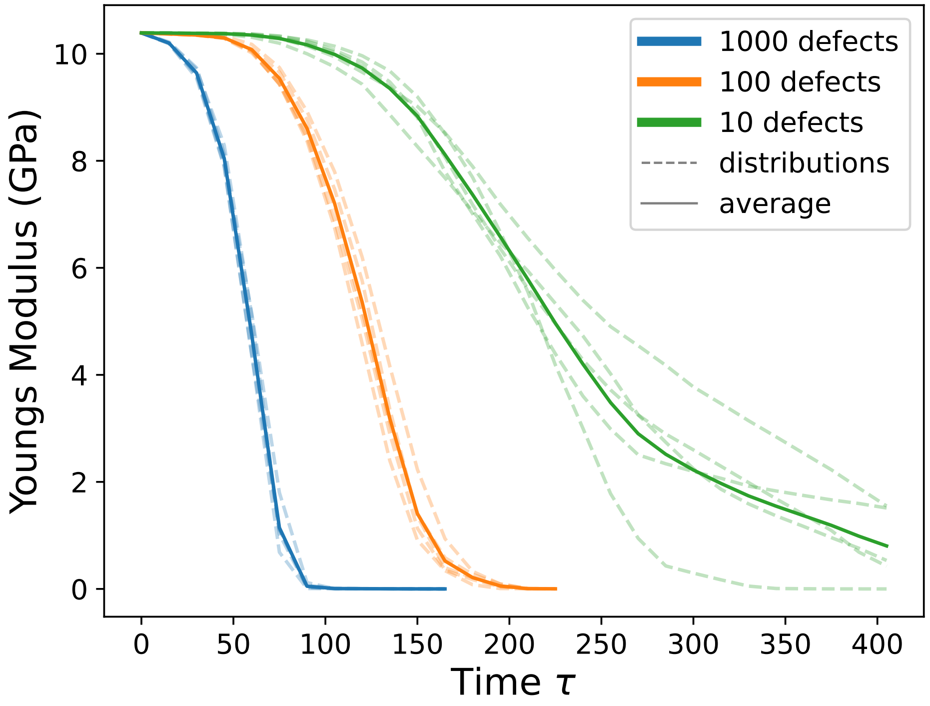
$E_{axial} = 230 \text{ GPa}, E_{radial} = 15 \text{ GPa}$

Young's modulus in fiber axis





Youngs's modulus across fiber

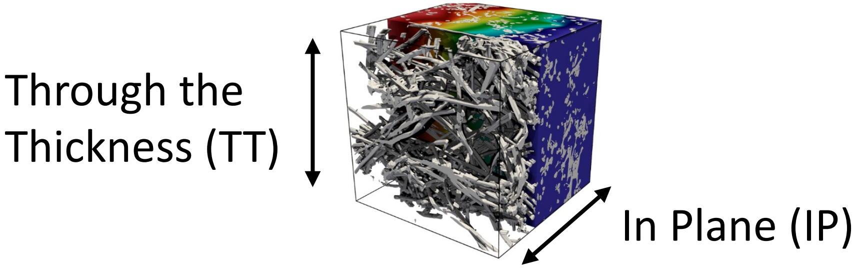


→ Stiffness degrades similar to thermal conductivity.

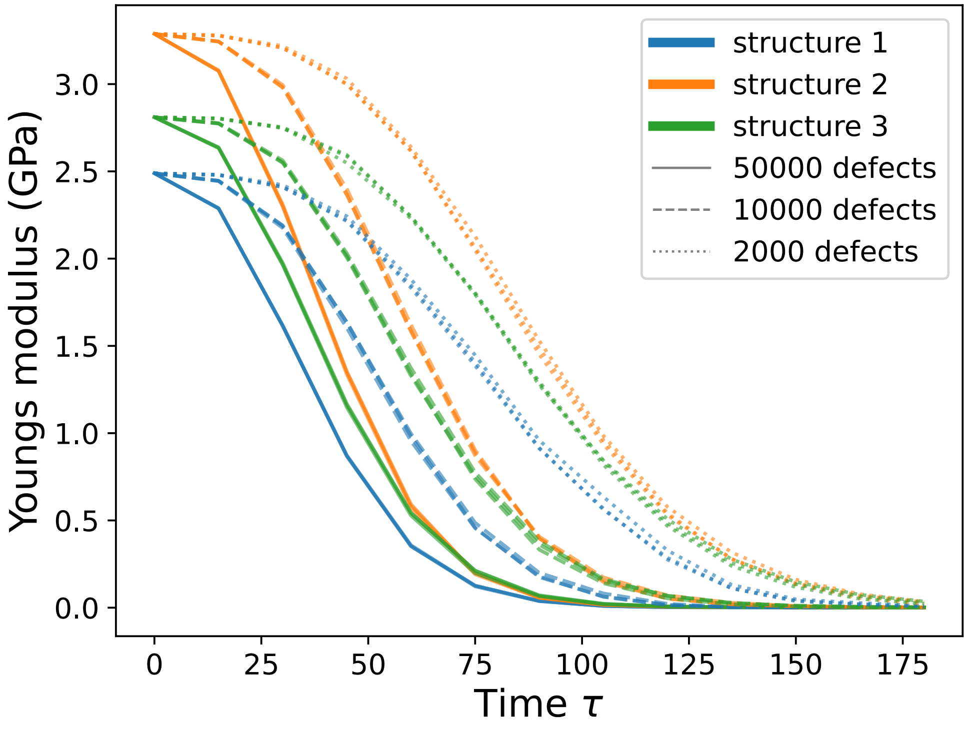
Linear Elasticity Results – FiberForm

Intrinsic fiber properties

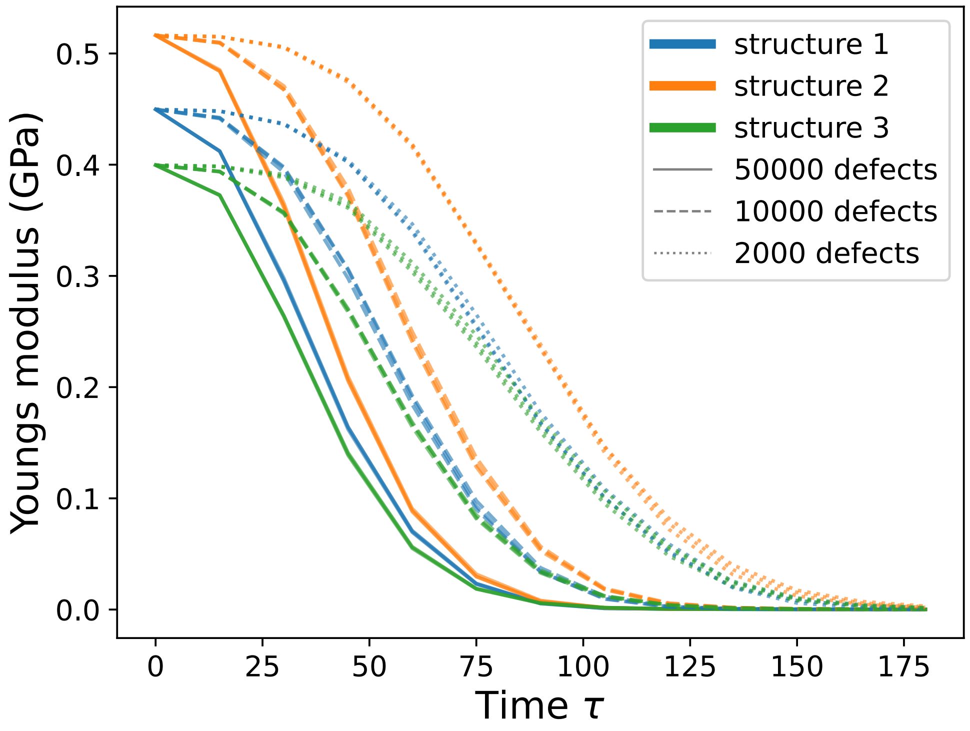
$E_{axial} = 230 \text{ GPa}, E_{radial} = 15 \text{ GPa}$



Youngs's Modulus IP

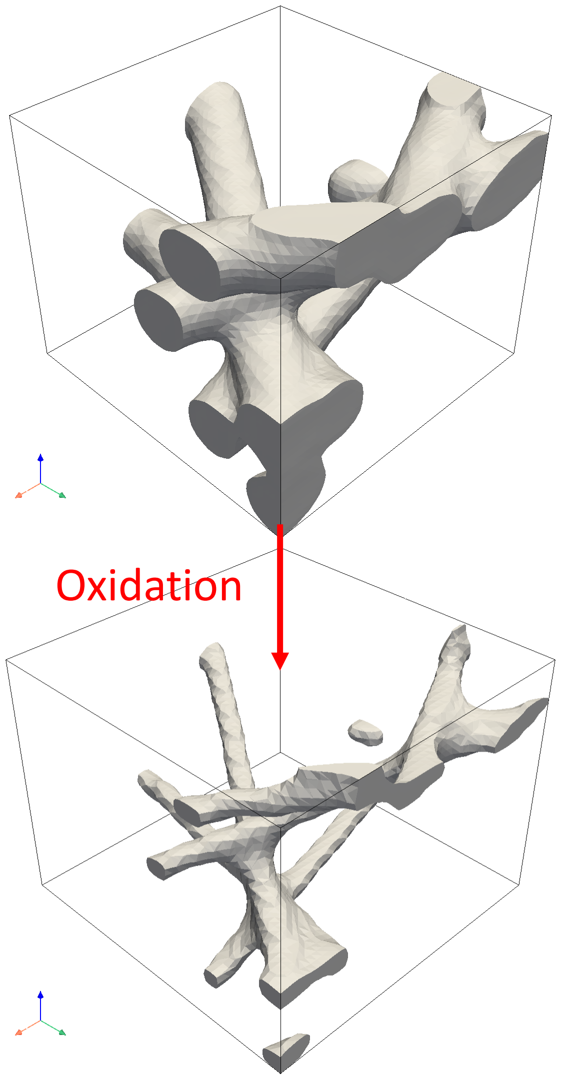


Young's Modulus TT

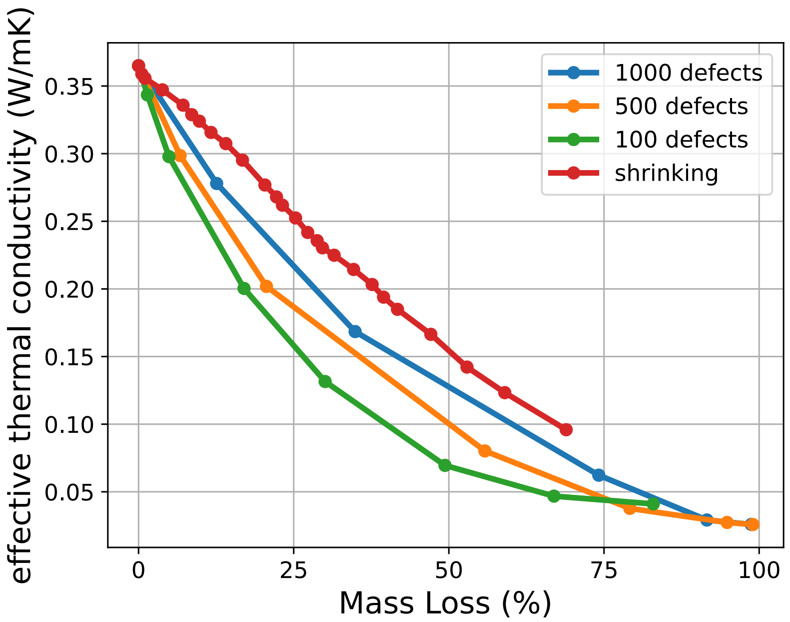


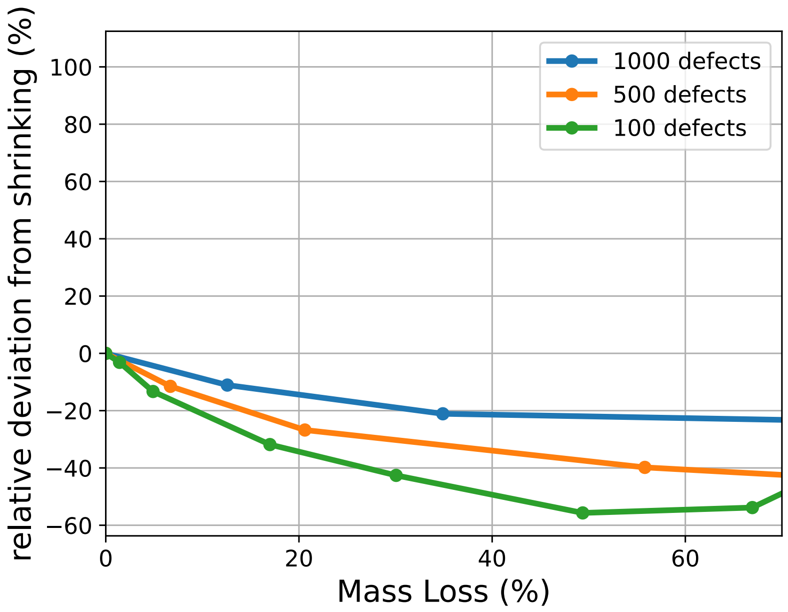
→ Stiffness degrades similar to thermal conductivity.

Comparison to legacy oxidation models



Legacy Model: Surface is consumed uniformly
→ shrinking fibers





Pitting model introduces nonlinear degradation
→ Thermal conductivity degrades much faster on a per mass basis

Key Takeaways

- Active-site-fraction feature was implemented in SPARTA to simulate pitting of carbon ablators in all relevant flight regimes
- PuMA has been utilized to observe degradation of material properties of single carbon fibers and carbon fiber microstructures
- Degradation due to pitting introduces nonlinear material behavior, unlike legacy shrinking model
- Pitting potentially introduces new failure mode due to fragmentation of fibers into chunks

Future Work:

- Fully homogenize results by simulating larger structures following Representative Volume Element (RVE) method
- Develop pitting model for effective material properties on macroscopic level

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