DSMC simulation of etch pit formation through active sites in carbon fiber microstructures

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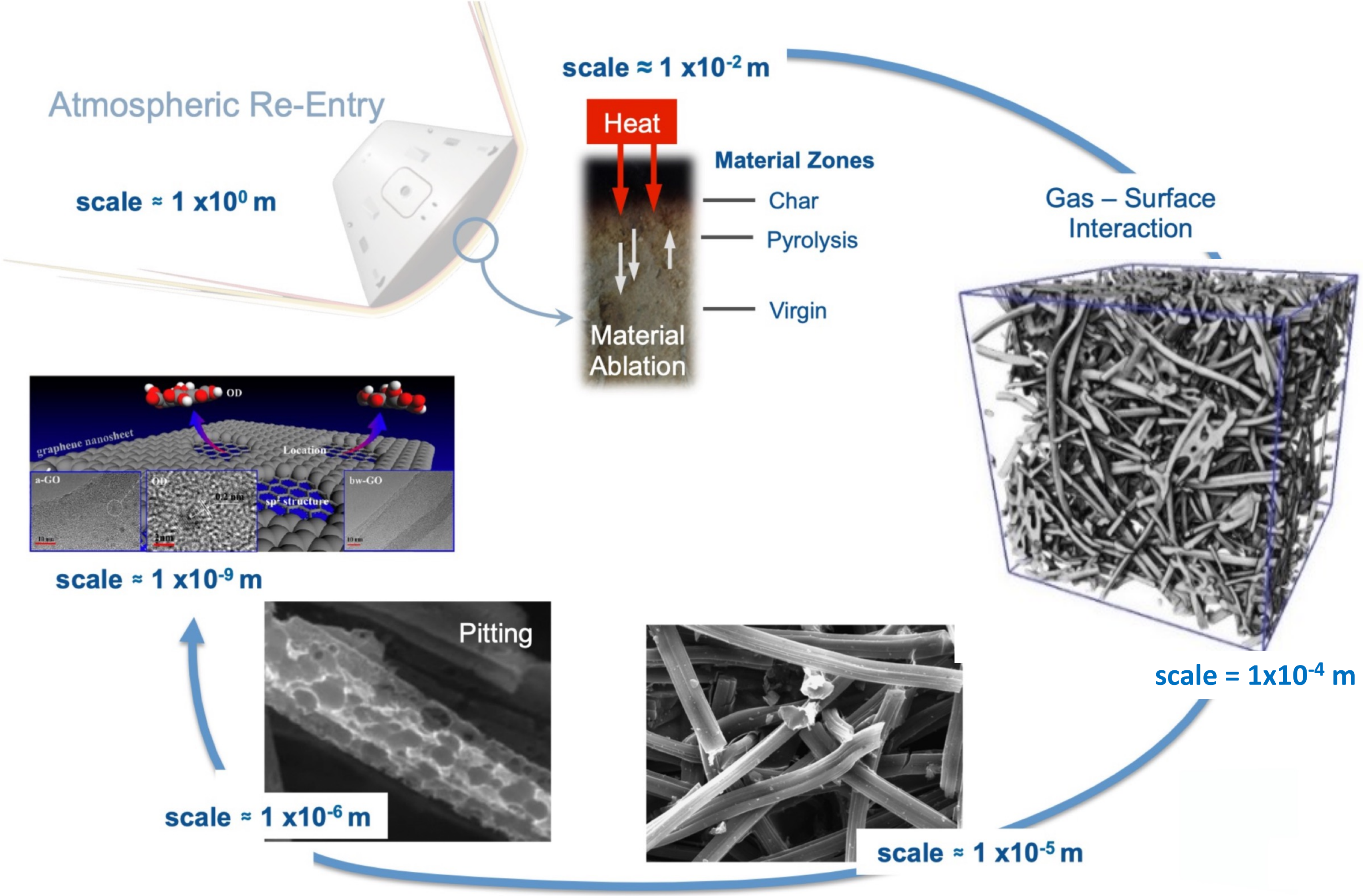
Motivation



Overall Objective:

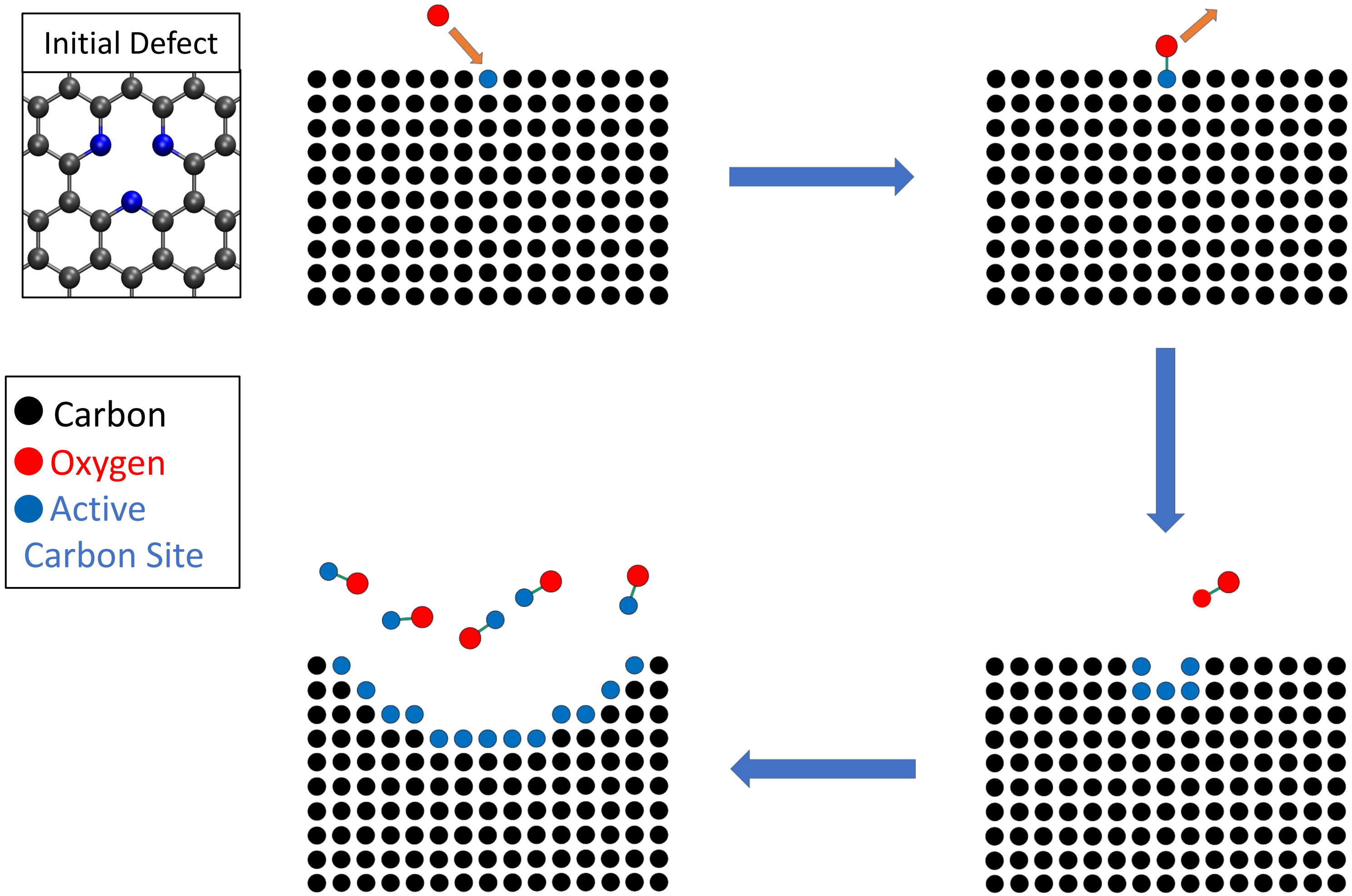
Model the degradation of carbon ablators due to oxidation and characterize their failure mechanisms.

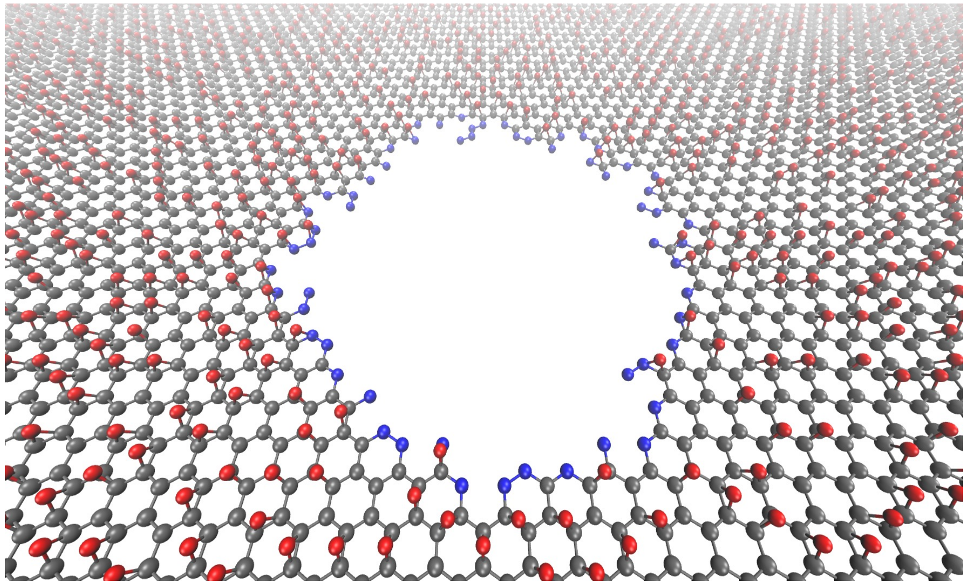
Current Work Objectives:

- Implement active-site capability in DSMC and capture the pitting process.
- Analyze the changes in reactivity due to active sites.

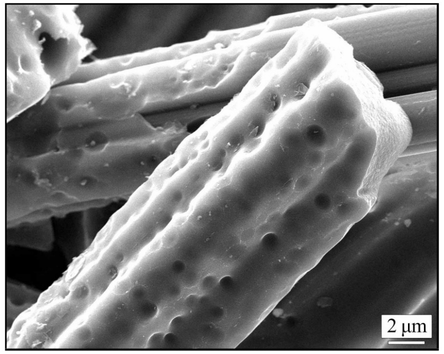
[1] F. Panerai, *et al*. In: Proceedings of the 44th AIAA Thermophysics Conference. 2013, pp. 1–14
[2] F. Panerai *et al*. In: International Journal of Heat and Mass Transfer 108 (2017), pp. 801–811. doi: 10.1016/j.ijheatmasstransfer.2016. 12.048.
[3] X. Chen and B. Chen. In: Environmental Science & Technology 50.16 (Aug. 2016), pp. 85688577

Pitting in Carbon Surface Oxidation





taken from [9]



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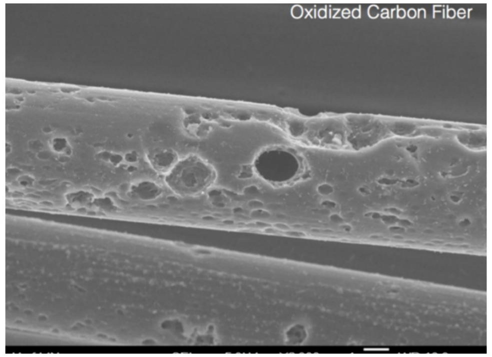
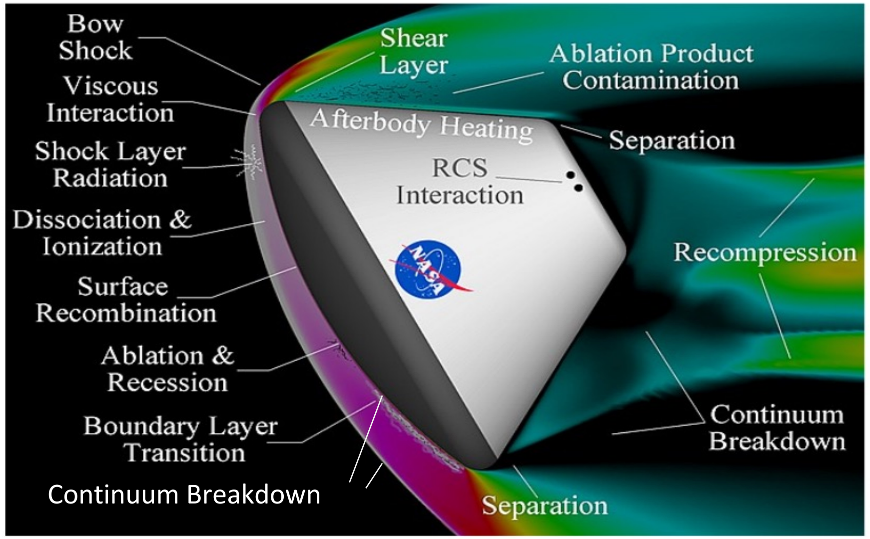


taken from [11]

[9] Simon Schmitt *(2020), PhD thesis.*
[10] Ringel, B. M., Panerai, F., Helber, B., Fagnani, A., & Turchi, A. (2022). In *AIAA AVIATION 2022 Forum* (p. 3947)
[11] Fu, R., Schmitt, S., & Martin, A. (2022). In *AIAA SCITECH 2022 Forum (p.1282)*

DSMC – SPARTA [4]

Continuum breakdown



DSMC

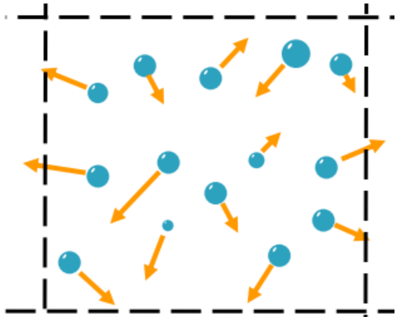
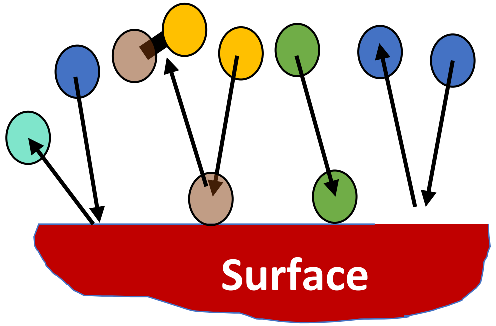


Image courtesy: https://prateekvjoshi.com/

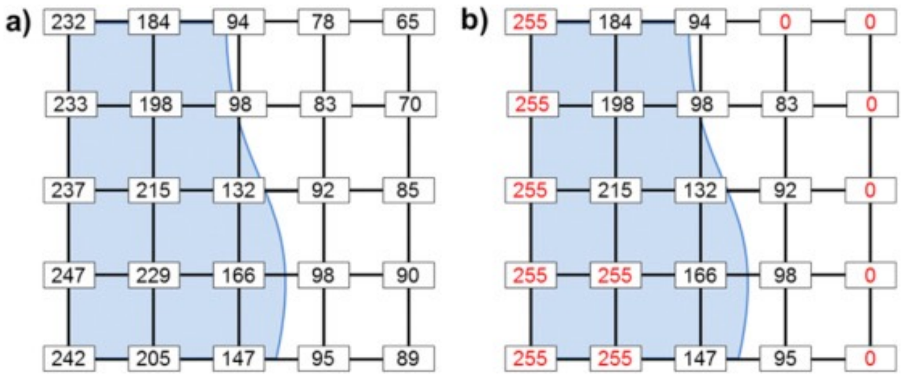


- CFD is not valid in regions of continuum breakdown
- DSMC (direct simulation Monte Carlo) is a stochastic, particle-based method to solve the Boltzmann equation
- DSMC is valid in all regimes: continuum, rarefied and transition (however computational cost increases with density)

[4] Plimpton, S. J., *et al*. "Direct simulation Monte Carlo on petaflop supercomputers and beyond." *Physics of Fluids* 31, no. 8 (2019): 086101.

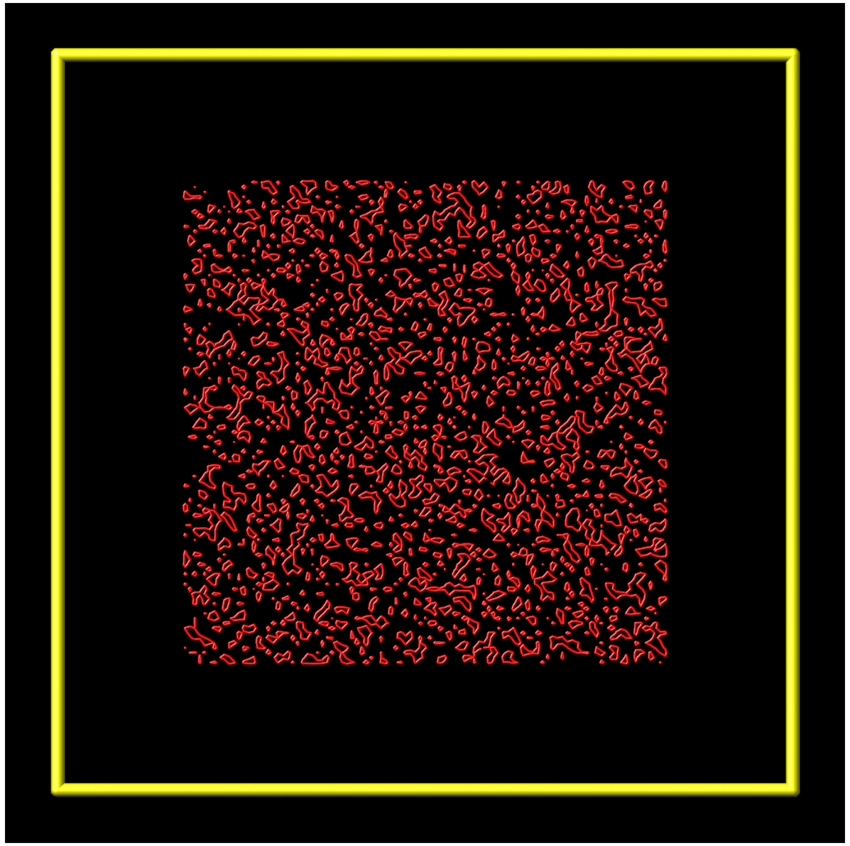
Ablation with implicit surfaces in SPARTA

- Geometry of individual elements inferred from 2D or 3D input file with pixel or voxel micro-CT data
- Choice of threshold determines solid-gas boundary



taken from [7]

- Triangulation of level-set surface computed by Marching Squares (MS; in 2D) or Marching Cubes (MC; in 3D) algorithms
- Up to 15 triangles per cell, entirely contained within grid cell
- MC is inherently parallel
- Implementation of MC in SPARTA includes topological and robustness enhancements to guarantee watertightness [8]

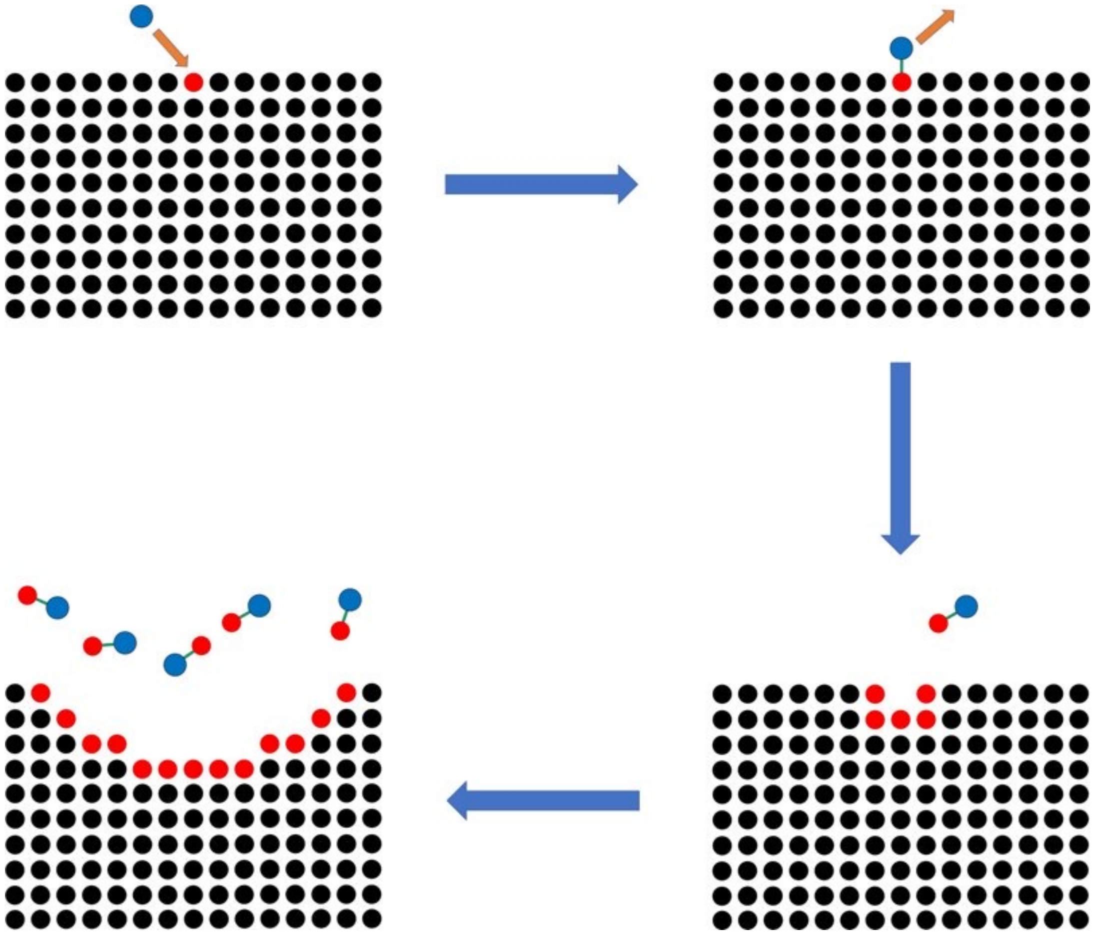


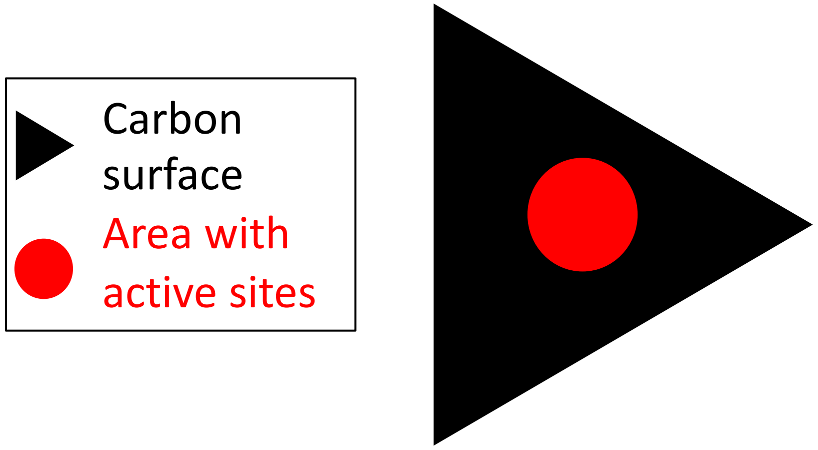
[7] Ferguson et al., Modeling the oxidation of low-density carbon fiber material based on micro-tomography. *Carbon* (2016)
[8] Custodio et. al, An extended triangulation to the Marching Cubes 33 algorithm. J. Braz. Comp. Soc. (2019)

Active Site Implementation in SPARTA

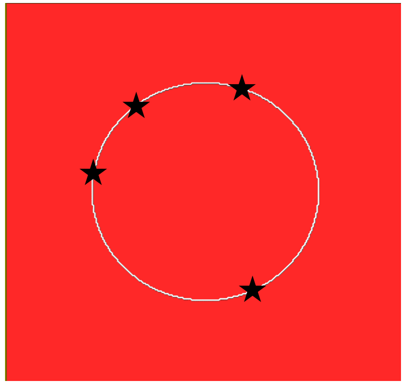
Guiding Principle:

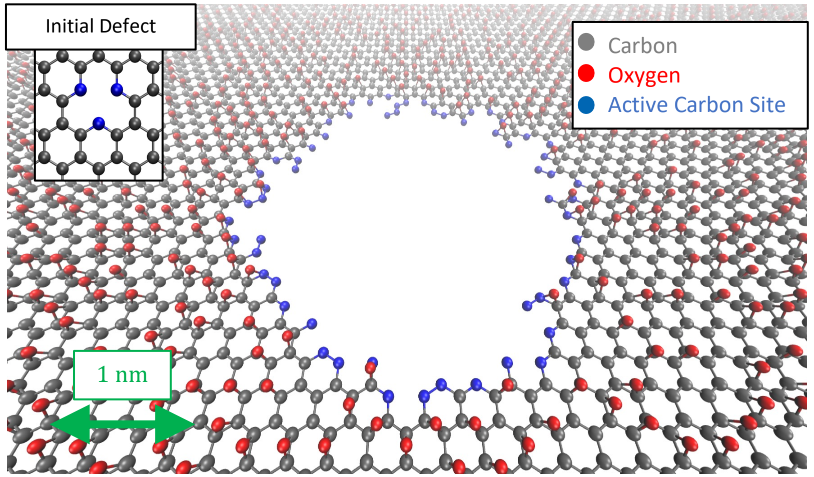
- New surface quantity called "active site fraction" (ASF) = fraction of surface element area with active sites
- Based on ASF, gas particles collide either with active or passive site
- Reactivity at active sites is much higher than at passive sites, and the reaction rate for oxidation (CO formation) is scaled accordingly





Active Site Implementation in SPARTA





taken from [9]

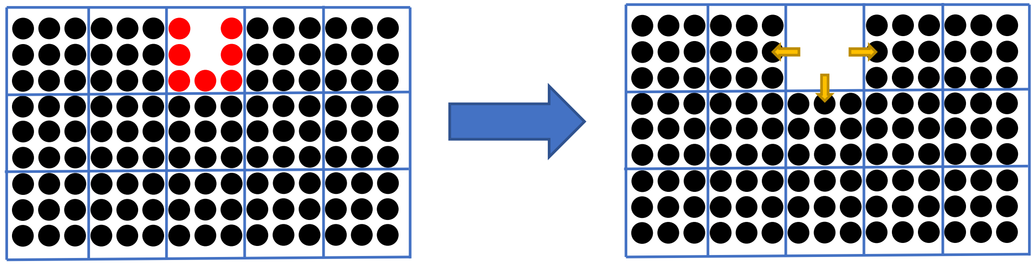
Methodology:

- Initialization
  - ❖ Defects are randomly distributed on a few surface elements based on user input defect density.
  - ❖ Active site fraction for these surface elements are set to a small number.

- Change in ASF (within a grid cell) due to reactions
  - ❖ This step is complex, as the increase or decrease of active sites due to a carbon removal depends on the actual geometry.
  - ❖ Currently ASF remains unchanged due to reactions.
  - ❖ Will use kMC simulations to get realistic values for change in ASF.

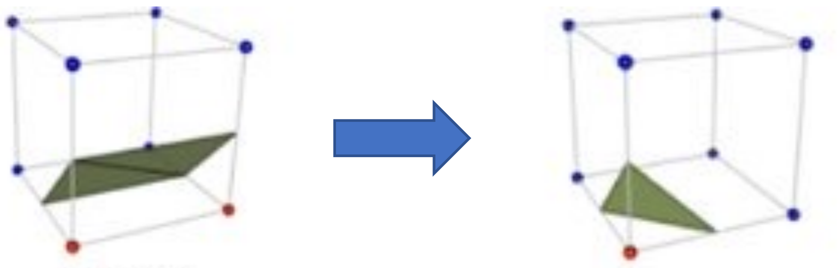
[9] Simon Schmitt *(2020), PhD thesis.*

Active Site Implementation in SPARTA



Methodology:

- Propagation to neighboring elements
  - ❖ When a grid cell is fully consumed (ablated), ASF of all neighboring elements are initialized to a small value.



taken from [8]

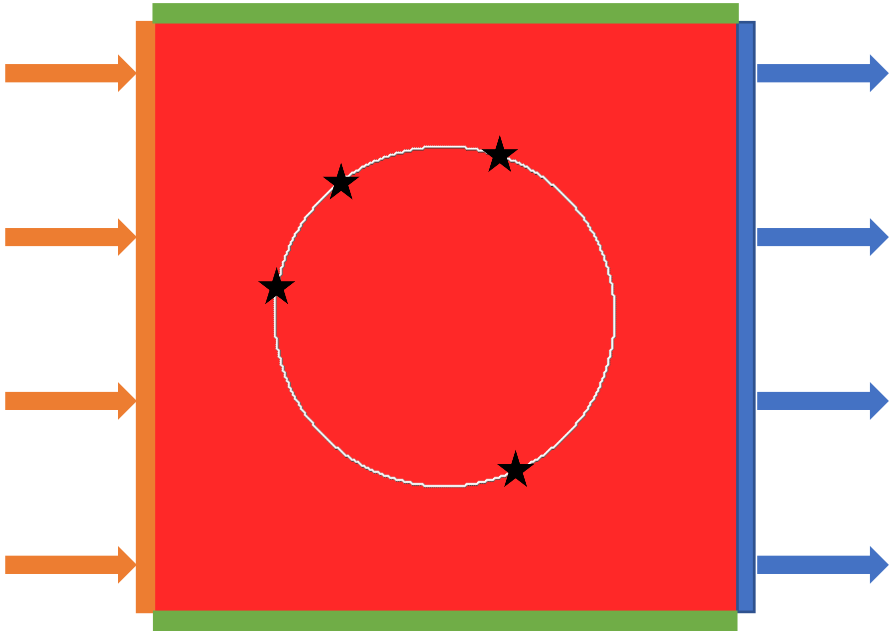
- Continuation through ablate step in DSMC
  - ❖ Before ablate – ASF of surface elements within a cell is averaged.
  - ❖ After ablate – ASF of new surface elements is set to this averaged value.

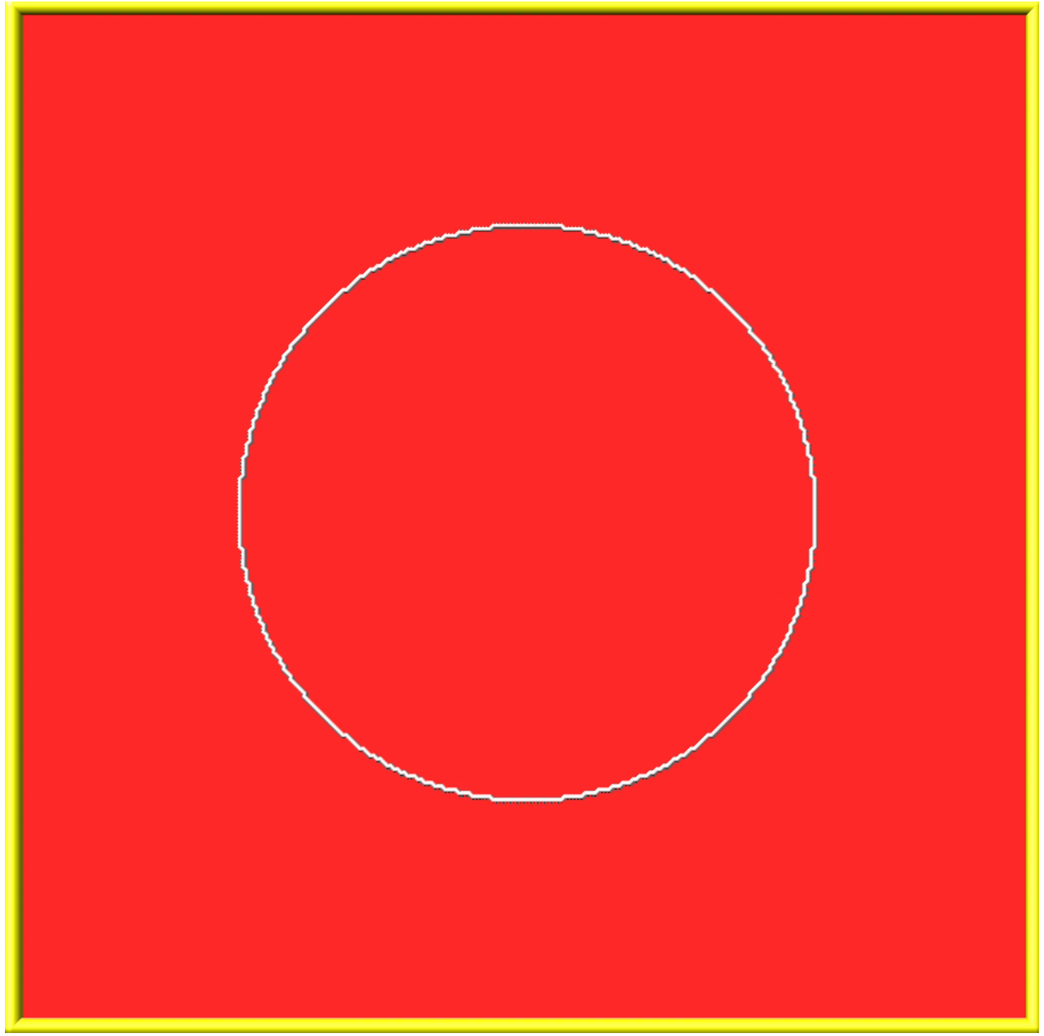
[8] Custodio et. al, An extended triangulation to the Marching Cubes 33 algorithm. J. Braz. Comp. Soc. (2019)

DSMC Results – 2D

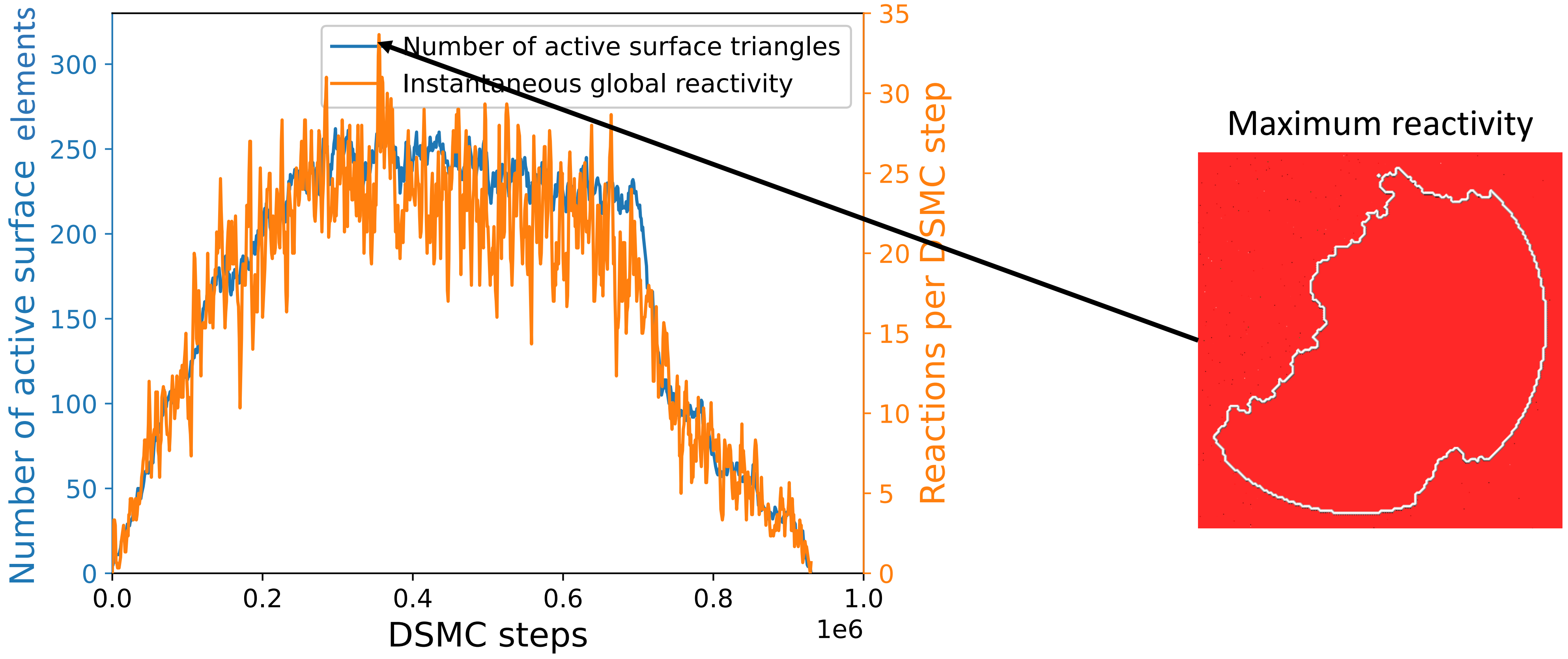
Simulation setup:

- Atomic Oxygen particle inflow
- O/CO particle outflow
- Periodic BC
- Initial active sites





Evolution of active surfaces vs reactions

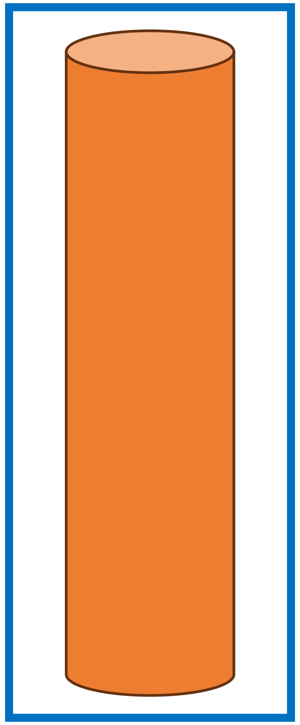


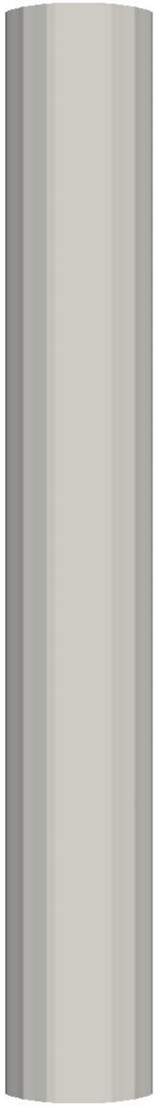
- Pitting causes nonlinear variation in reactivity due to active site evolution and flow-geometry interactions

Pitting Simulation Results – Single Fiber

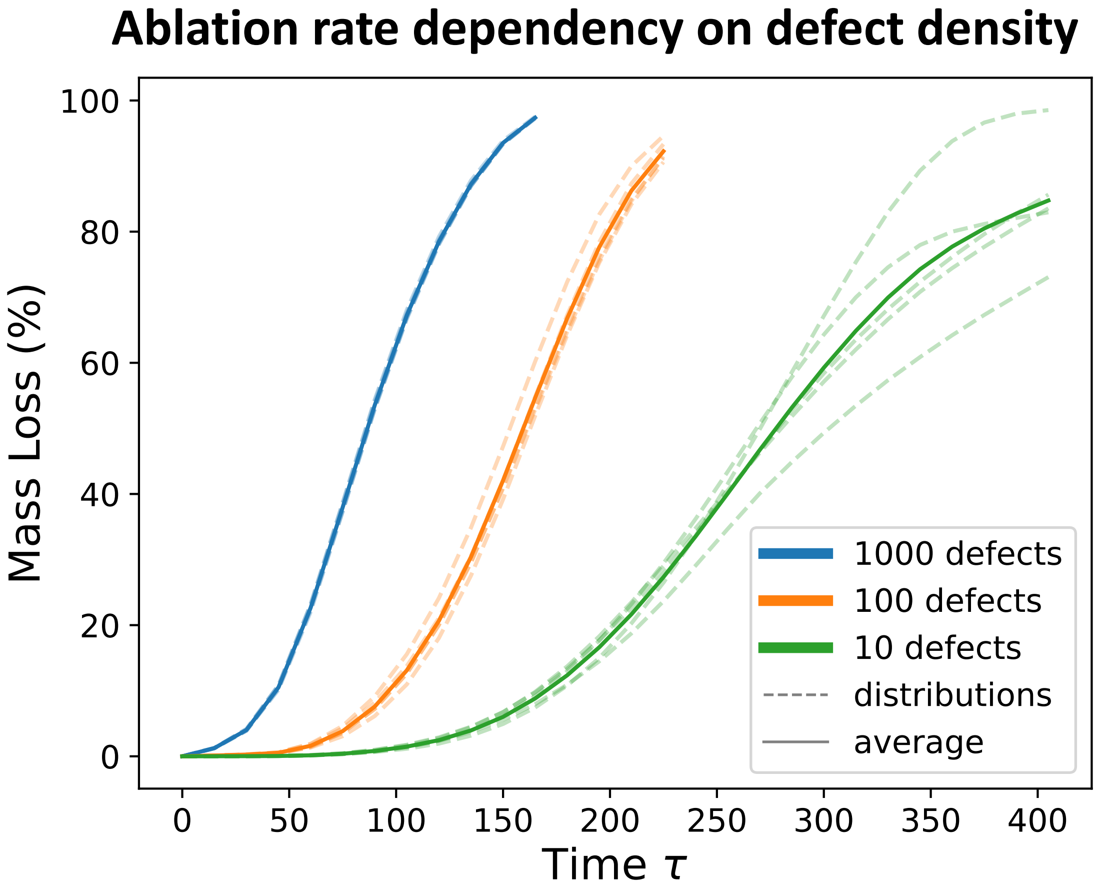
Simulation setup:

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





Pitting Simulation Results – Single Fiber

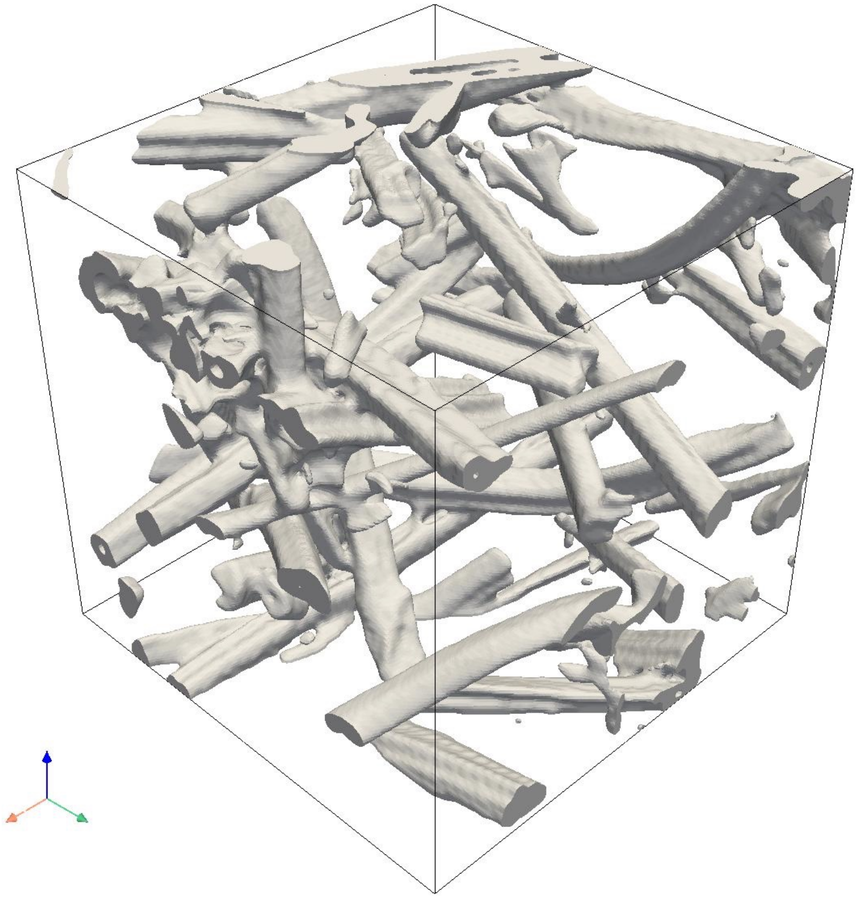


- Pitting fragments fiber into chunks
- Higher number of pits cause faster ablation
- Variance with pit distribution is inversely related to number of pits

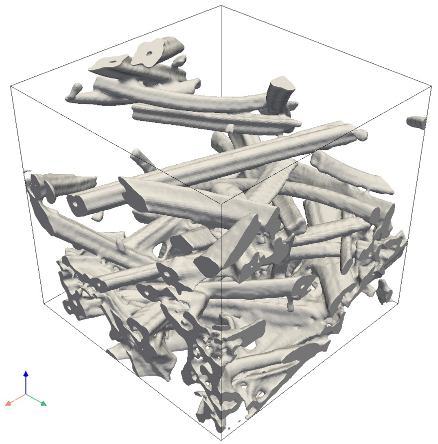
Pitting Simulation Results – FiberForm

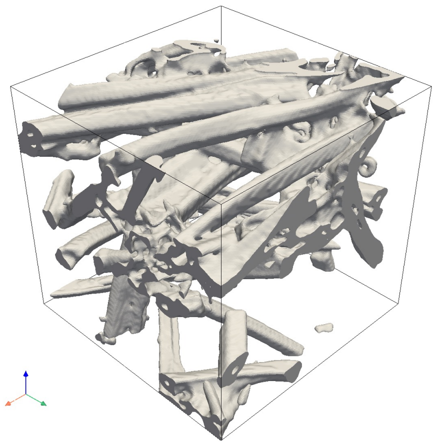
Simulation setup:

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

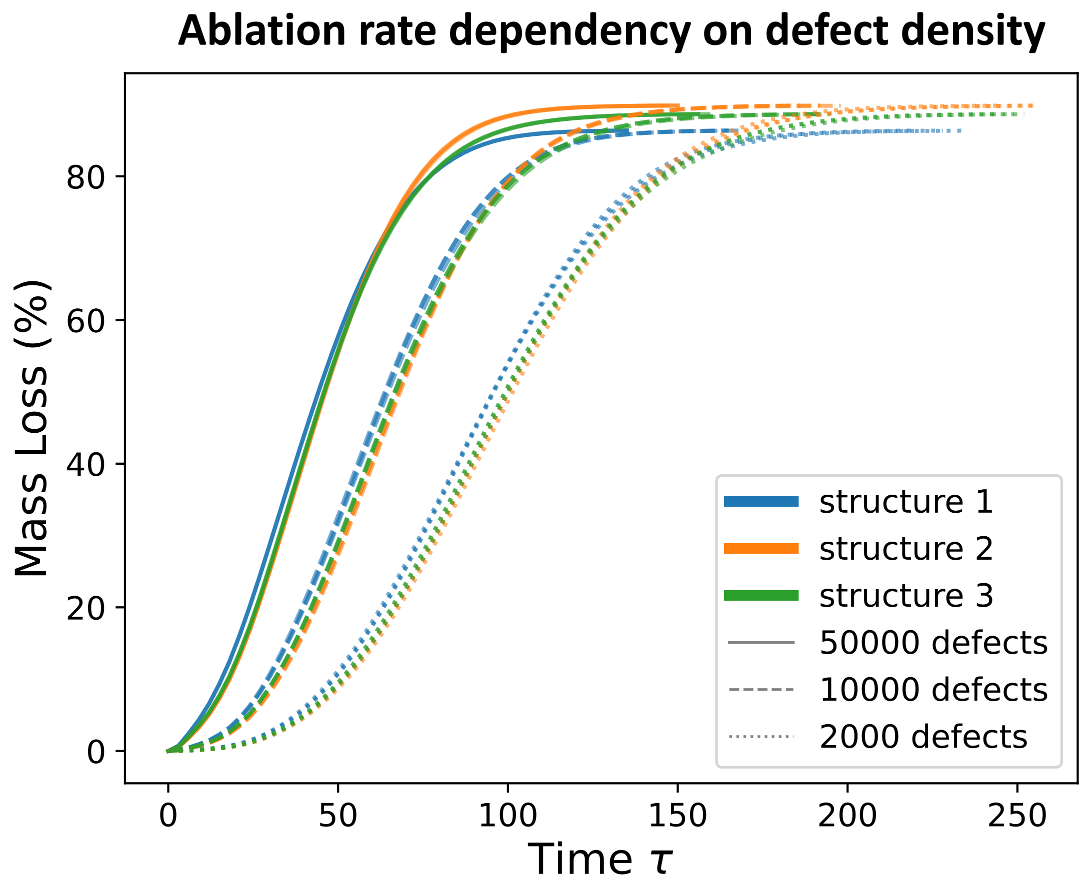


Other Substructures





Pitting Simulation Results – FiberForm



- Higher the number of defects/active sites, faster the ablation.
- Variance with pit distribution generally very low.
- Variance between different substructures is also low.

Summary

- Active-site-fraction feature was implemented in DSMC code SPARTA to simulate the formation of etch pits due to oxidation of carbon ablators.
- Simulations of pitting were performed for a single fiber and FiberForm.
  - ❖ Reactivity is directly linked to the active surface elements.
  - ❖ Pitting causes nonlinear variation in reactivity due to active site evolution and flow-geometry interactions.
  - ❖ Pitting fragments fiber into chunks.
- Effect of the defect density and structure variation was also investigated.
  - ❖ Total ablation time decreases with increasing number of defects.
  - ❖ Variance with pit distribution is inversely related to number of pits.
  - ❖ Larger structures has smaller variance with pit distribution.
  - ❖ Different fiber substructures also have low variance in the total ablation time.

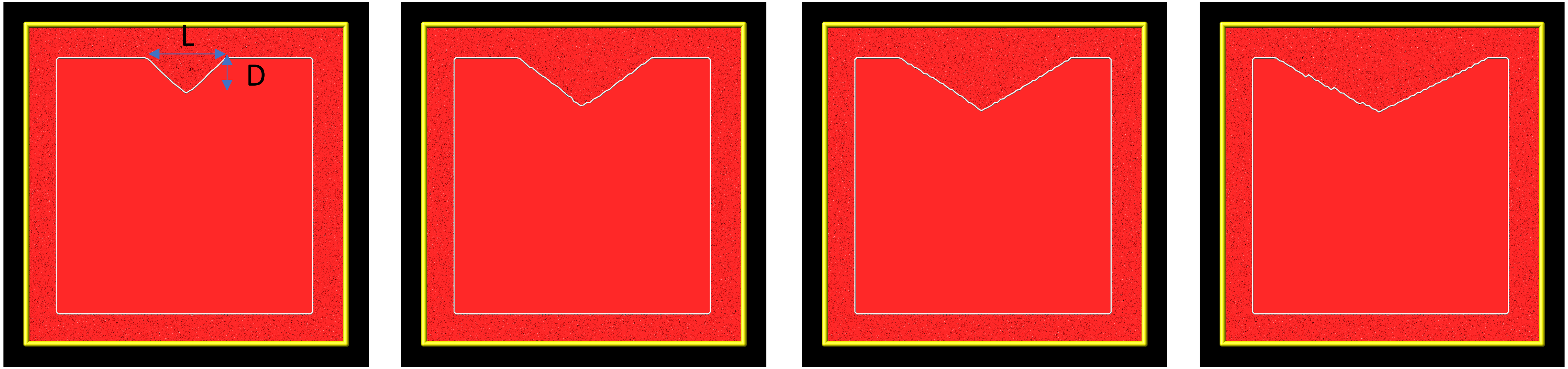
Future Work

Improve active-site feature in SPARTA to be more physically accurate.

- Change in ASF within a grid cell due to reactions
  - ➢ Currently performing kMC simulations to get realistic values.
- Propagation to neighboring elements
  - ➢ Pits grow faster in the in-plane direction than the in-depth direction.
  - ➢ Propagate the pits in the in-plane direction before the cell is fully depleted.

In-plane propagation at a cell depletion of

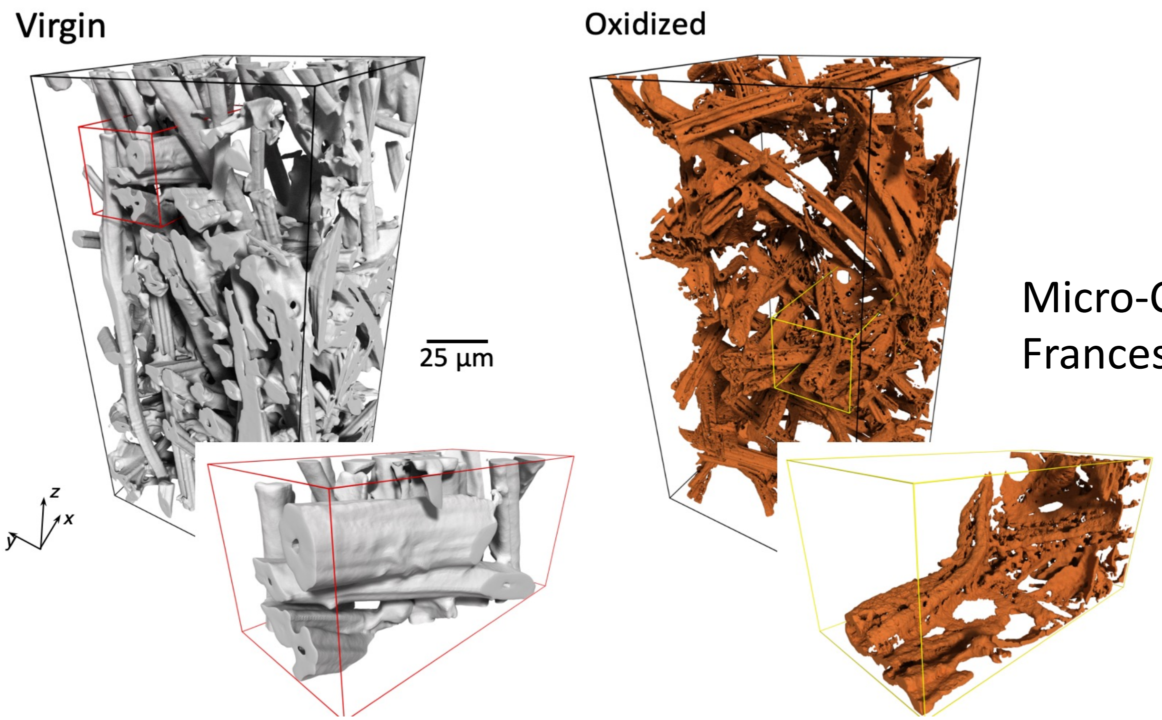
90% 85% 80% 75%



In-depth propagation at a cell depletion of 90%

Future Work

- Compare pitted FiberForm structures from SPARTA with experiments
- Analyze the distribution of pit sizes and growth rates of the pits.



Micro-CT data from Francesco Panerai

Thank You
Questions?

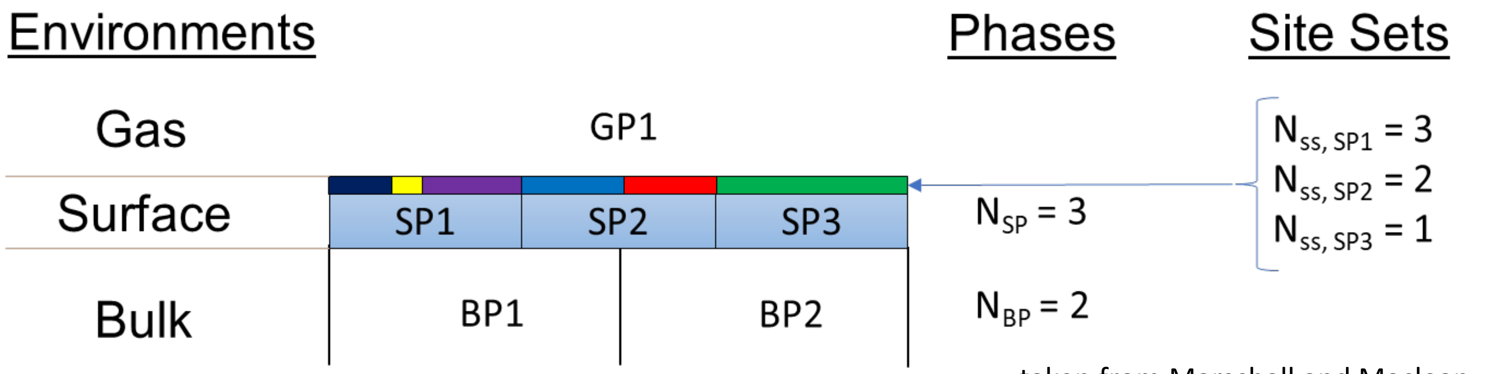
National Aeronautics and Space Administration

Ames Research Center
Entry Systems and Technology Division

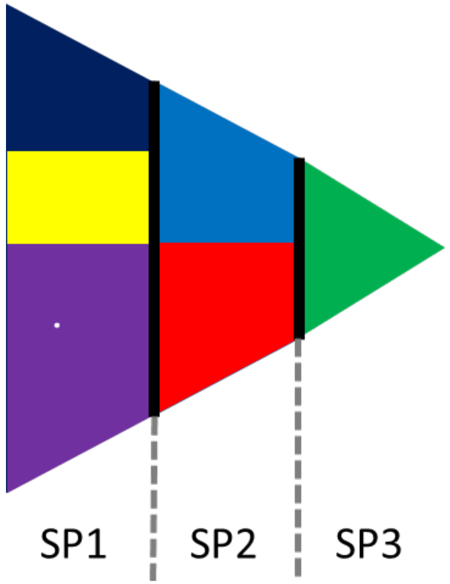
Backup Slides

Surface chemistry framework in DSMC [5]

- Methodology to represent surface sites similar to Marschall, Maclean and Driver [6] for CFD.
- Particles adsorb (deleted) and desorb (created) on the surface, surface element stores adsorbed particle concentration.
- Surface reactions based on concentration within surface element.
- Multiple triangulated elements (like cells) on surfaces
- Langmuir model for surface sites.

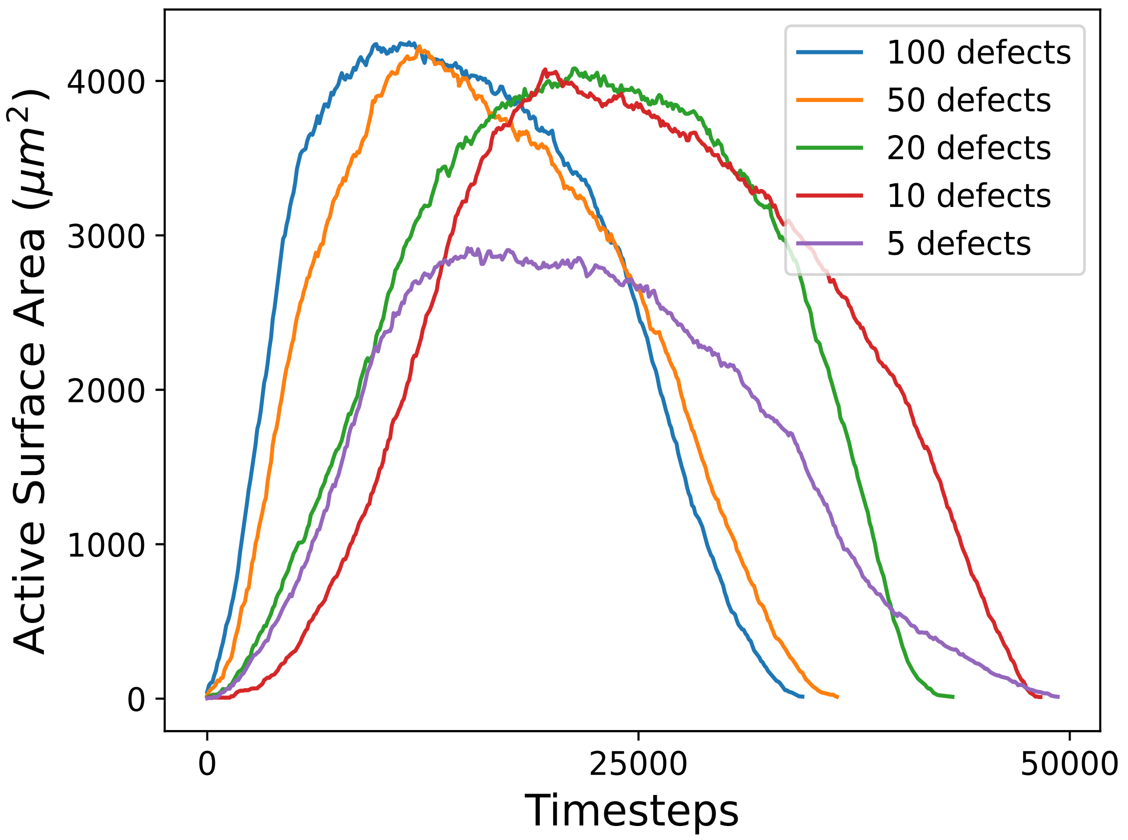


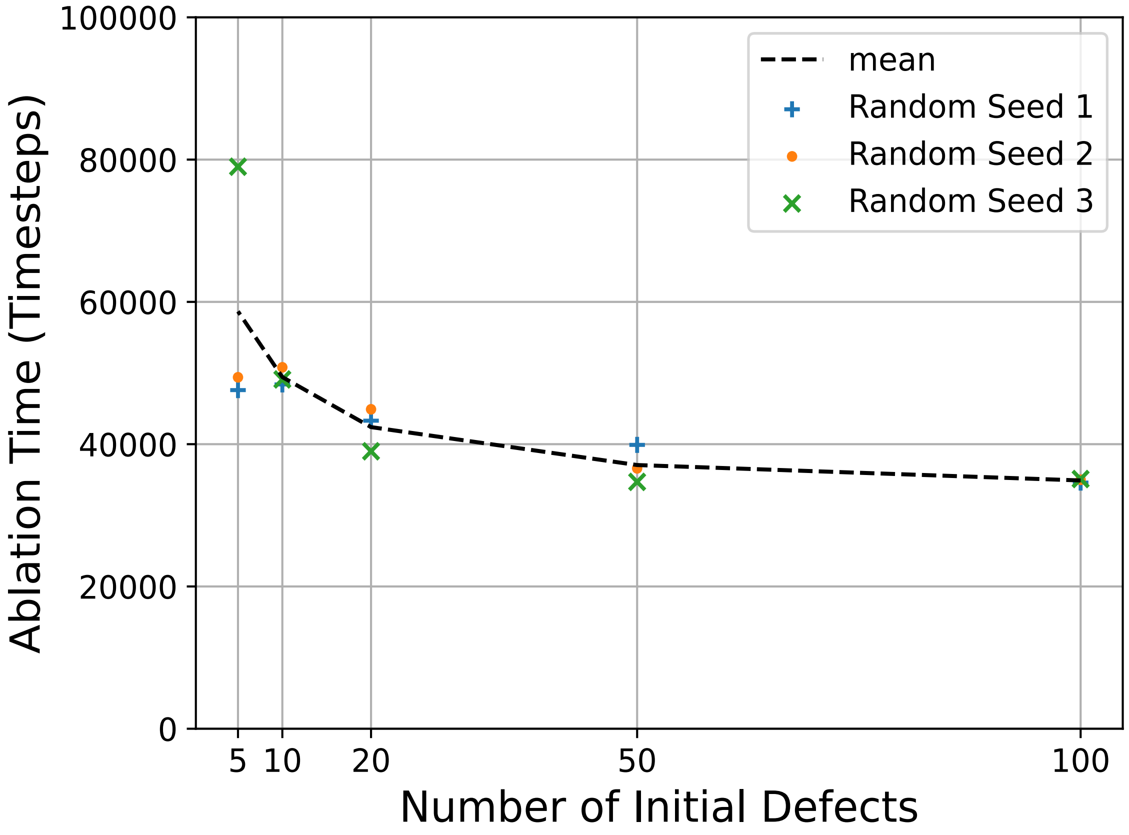
taken from Marschall and Maclean.



[5] Swaminathan Gopalan, K., & Stephani, K. A. (2018). **Development of a detailed surface chemistry framework in DSMC**. In 2018 AIAA Aerospace Sciences Meeting (p. 0494).
[6] Marschall, J., & MacLean, M. (2011). Finite-rate surface chemistry model, I: Formulation and reaction system examples. AIAA Paper, 3783, 2011.

Total ablation time



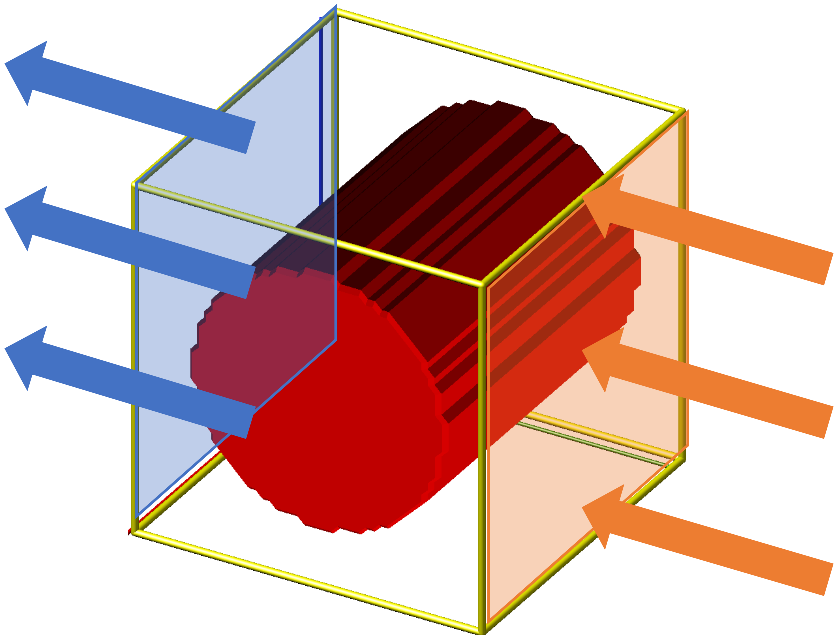


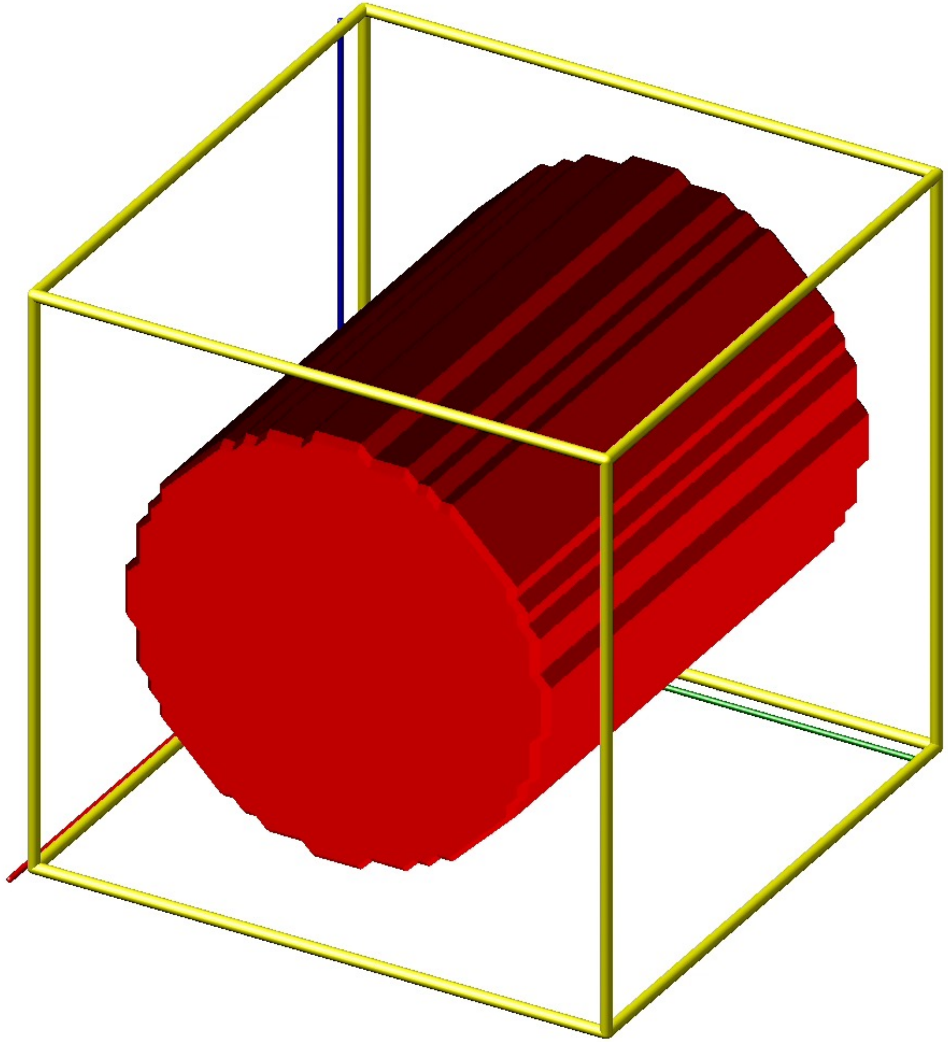
- Total ablation time decreases with increasing number of defects.

DSMC Results – 3D

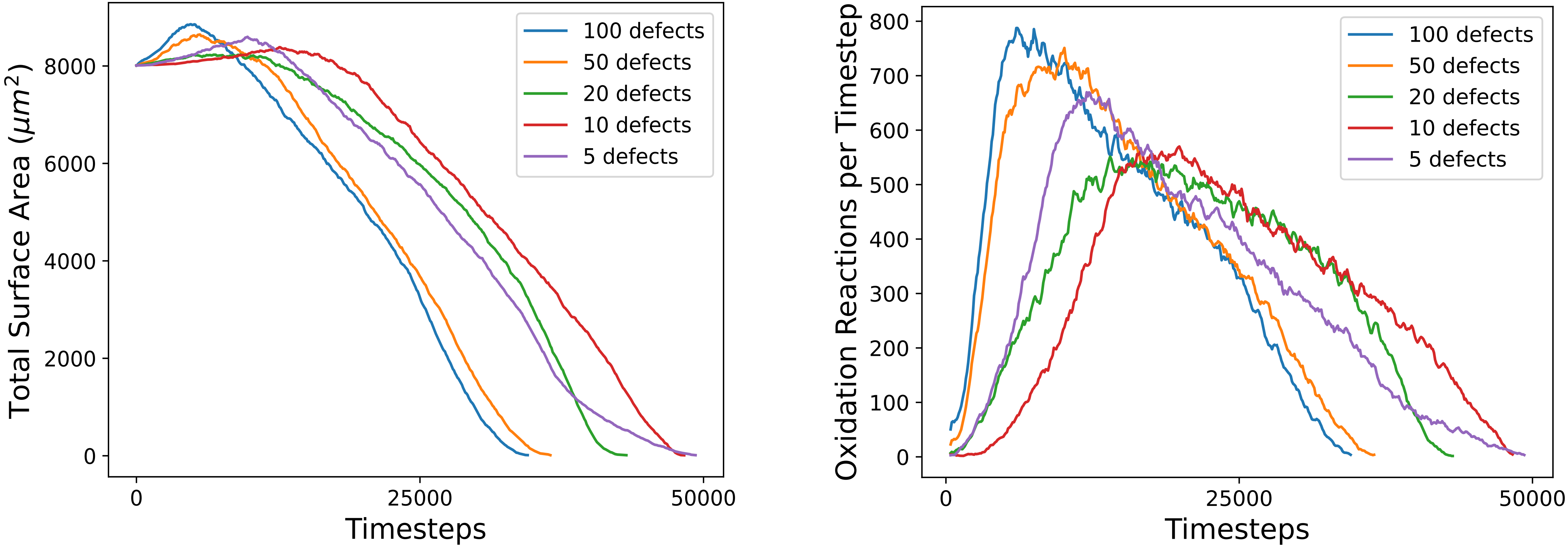
Simulation setup:

- Atomic Oxygen particle inflow
- O/CO particle outflow
- Periodic BC everywhere else
- Random distribution of initial active sites



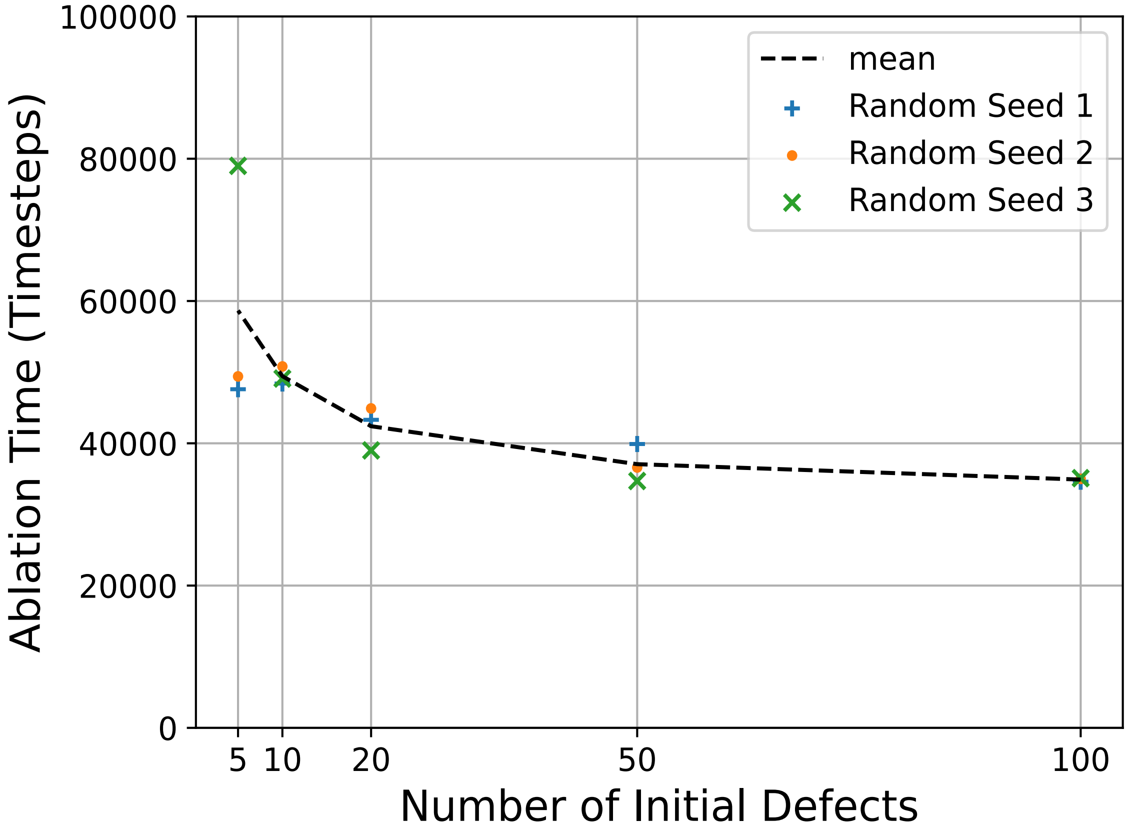


Effect of defect density



- Total surface area initially increases with material removal.
- Peak in reactivity occurs earlier with increasing number of defects.
- Reactivity decreases after the peak due to decreasing surface area.

Total ablation time



- Total ablation time decreases with increasing number of defects.