Implementation of active sites in DSMC to capture pitting of oxidizing carbon materials

Simon Schmitt, Krishnan Swaminathan Gopalan, and Arnaud Borner

Analytical Mechanics Associates Inc.

Thermal Protection Materials Branch, NASA Ames Research Center, Moffett Field, CA, 94035, USA

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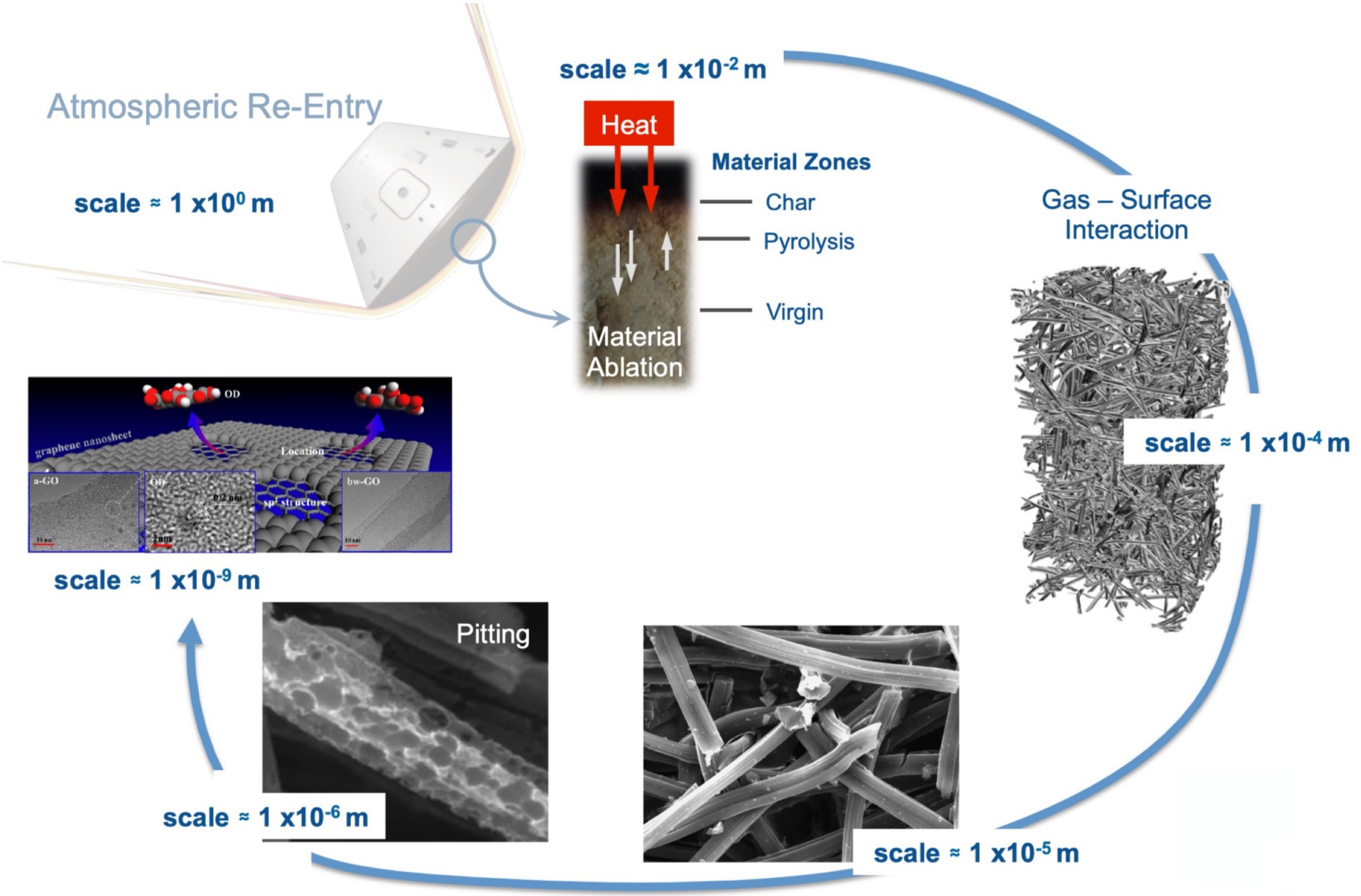
Motivation



Overall Objective:

Characterize the formation of etch pits on the FiberForm surface and their effect on its material properties

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

DSMC – SPARTA [4]

Continuum breakdown

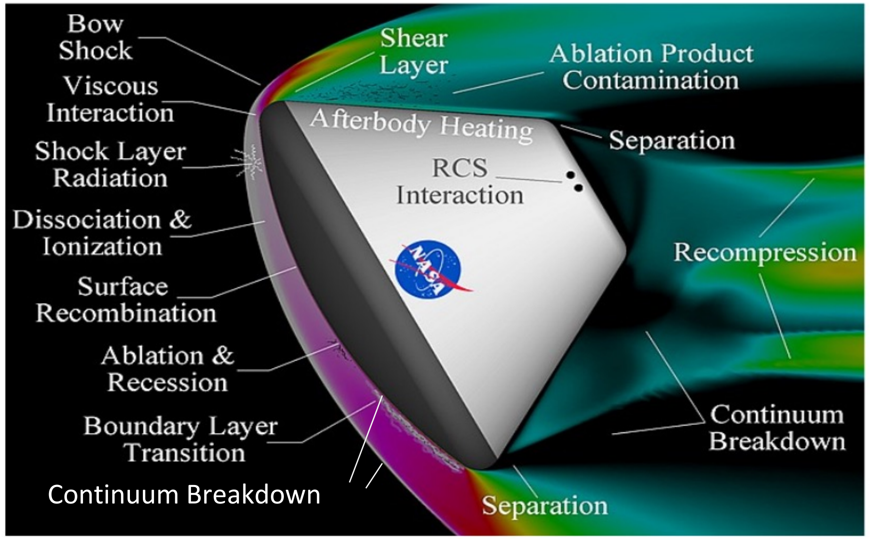


Image Credit: NASA

DSMC

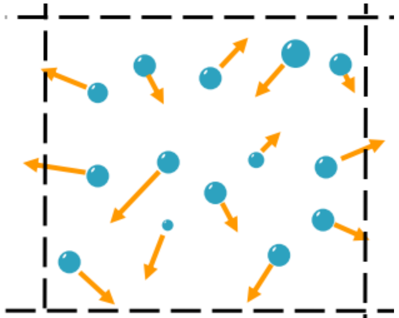
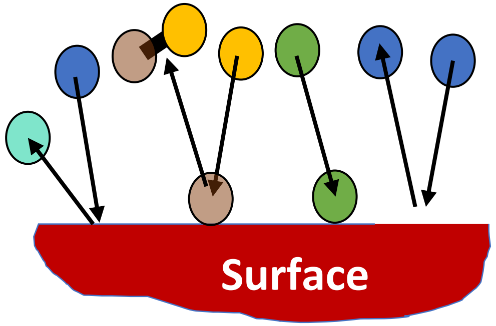


Image courtesy: https://prateekvjoshi.com/

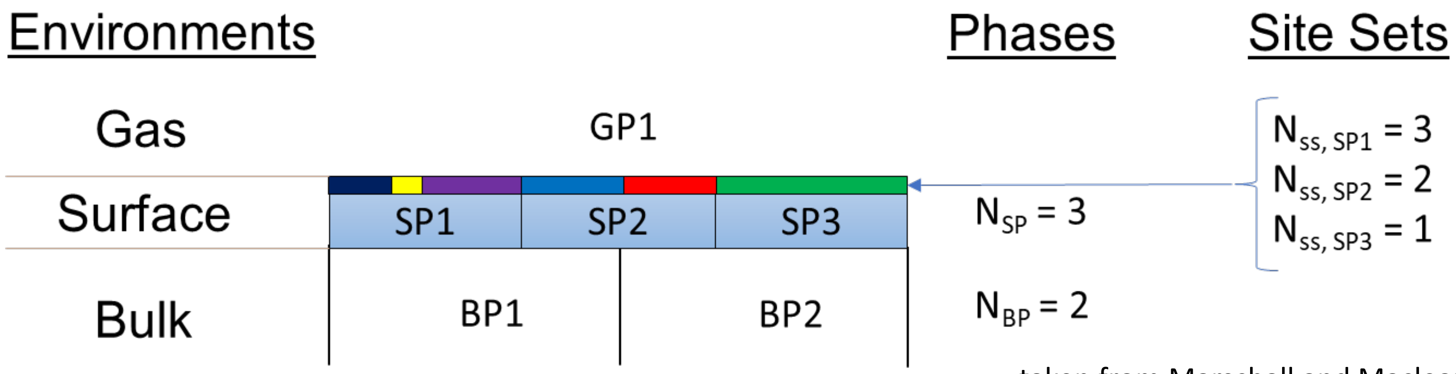


- CFD is not valid in regions of continuum breakdown
- DSMC (direct simulation Monte Carlo) is a stochastic, particle-based method to solve the Boltzmann equation
- DSMC is valid in all regimes: continuum, rarefied and transition (however computational cost increases with density)

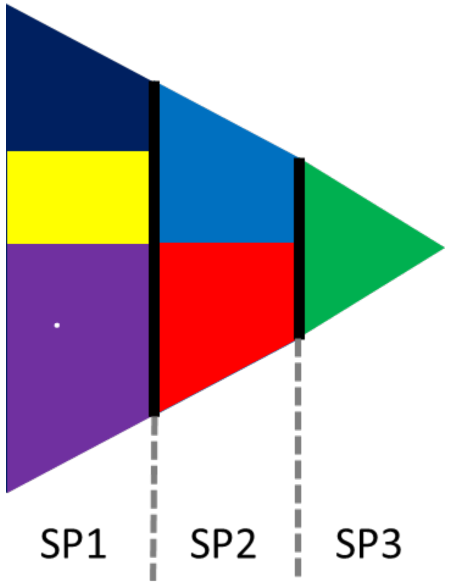
[4] Plimpton, S. J., *et al*. "Direct simulation Monte Carlo on petaflop supercomputers and beyond." *Physics of Fluids* 31, no. 8 (2019): 086101.

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.



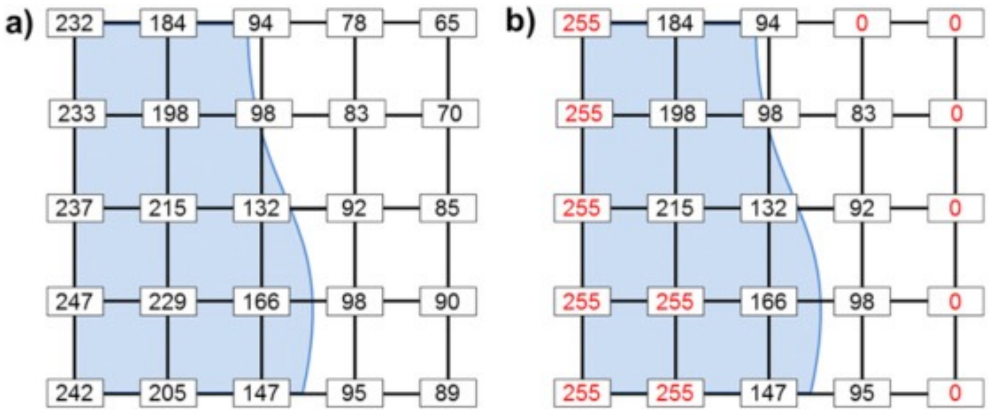
taken from Marschall and Maclean.



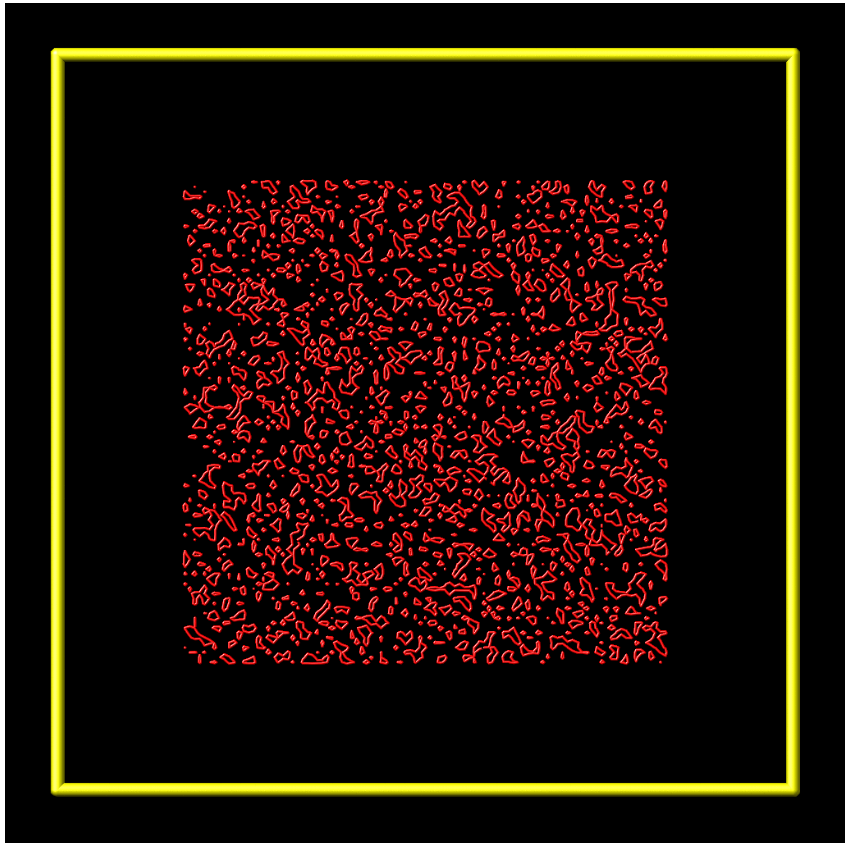
[5] Swaminathan Gopalan, K., & Stephani, K. A. (2018). **Development of a detailed surface chemistry framework in DSMC**. In 2018 AIAA Aerospace Sciences Meeting (p. 0494).
[6] Marschall, J., & MacLean, M. (2011). Finite-rate surface chemistry model, I: Formulation and reaction system examples. AIAA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

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

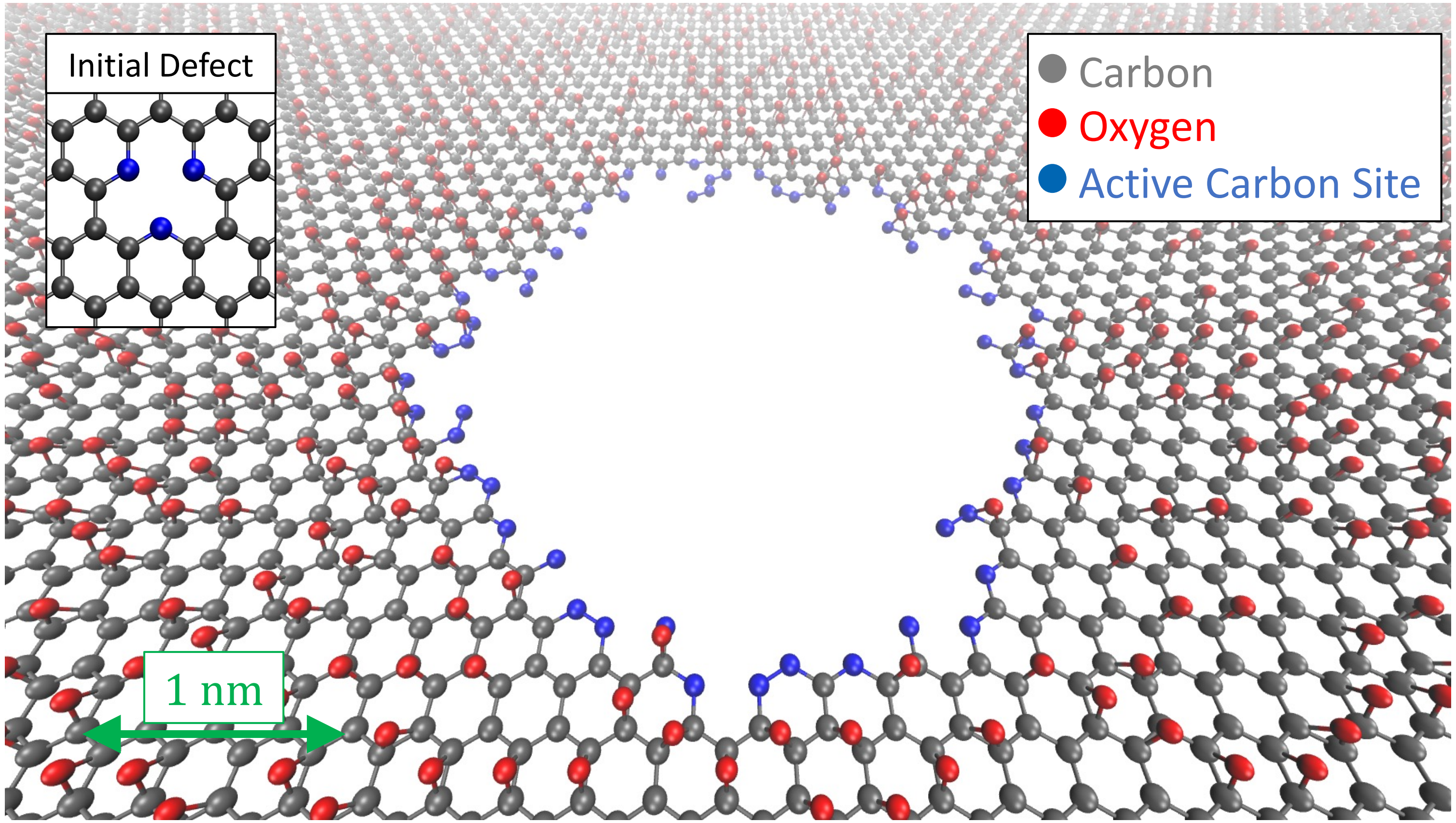


- Triangulation of level-set surface computed by Marching Squares (MS; in 2D) or Marching Cubes (MC; in 3D) algorithms
- Up to 15 triangles per cell, entirely contained within grid cell
- MC is inherently parallel
- Implementation of MC in SPARTA includes topological and robustness enhancements to guarantee watertightness [10]

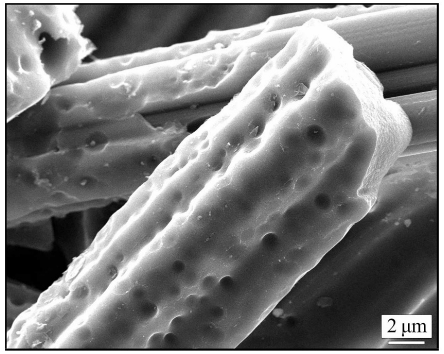


[10] Custodio et. al, An extended triangulation to the Marching Cubes 33 algorithm. J. Braz. Comp. Soc. (2019)

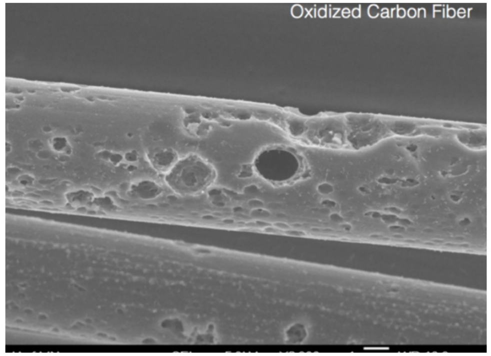
Pitting in Carbon Surface Oxidation



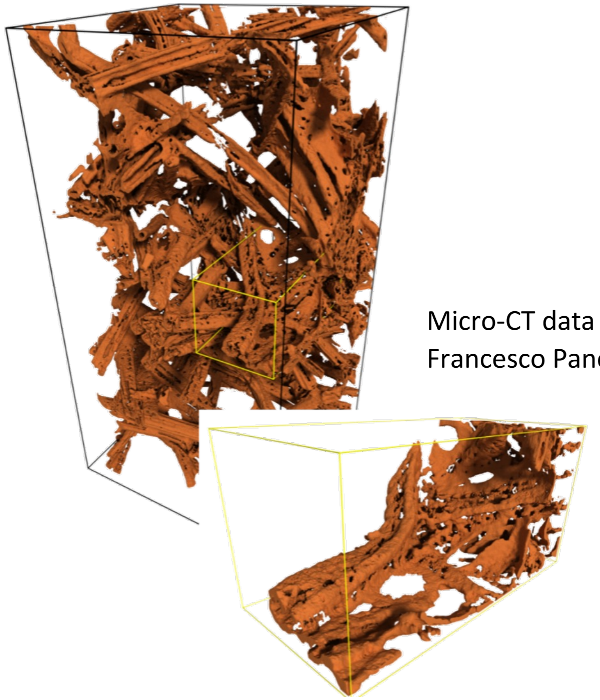
taken from [7]



taken from [8]



taken from [9]



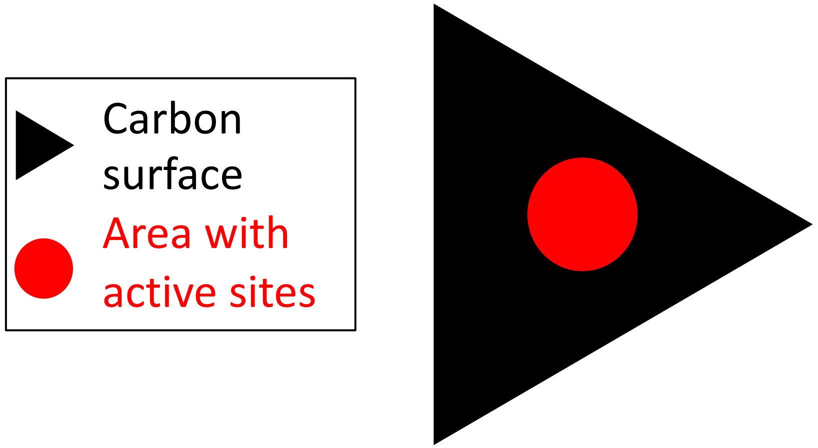
Micro-CT data from
Francesco Panerai

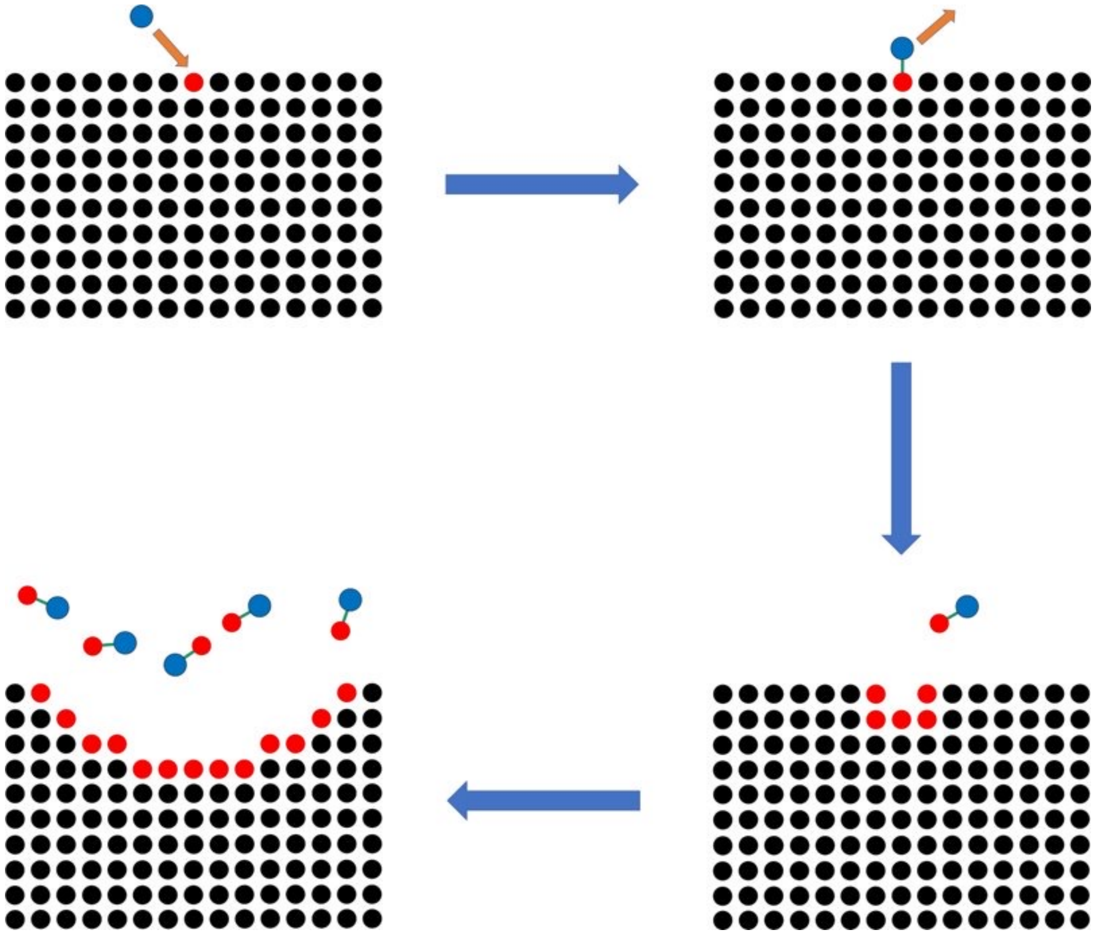
[7] Simon Schmitt *(2020), PhD thesis.*
[8] Ringel, B. M., Panerai, F., Helber, B., Fagnani, A., & Turchi, A. (2022). In *AIAA AVIATION 2022 Forum* (p. 3947)
[9] Fu, R., Schmitt, S., & Martin, A. (2022). In *AIAA SCITECH 2022 Forum (p.1282)*

Active Site Implementation in SPARTA

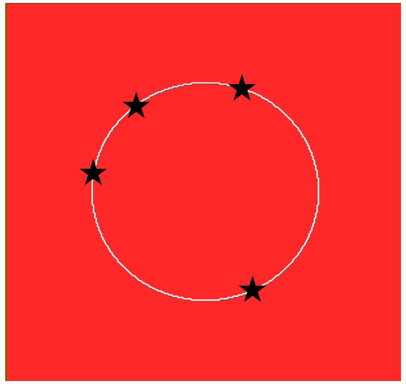
Guiding Principle:

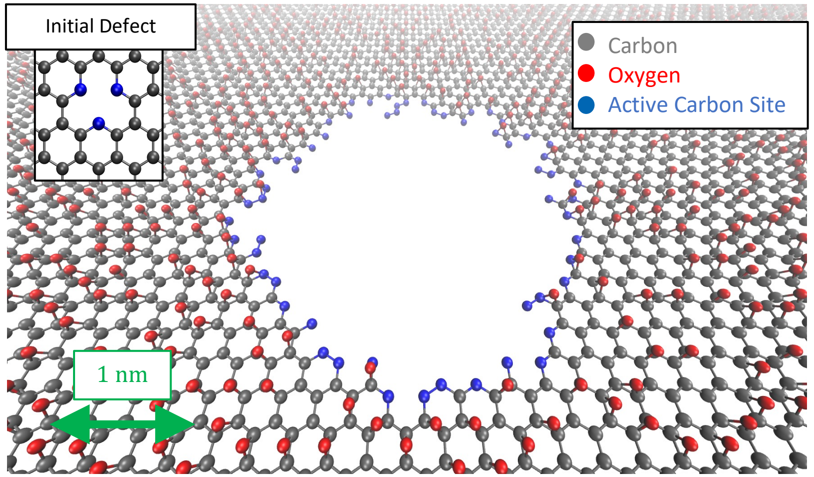
- New surface quantity called "active site fraction" (ASF) = fraction of surface element area with active sites
- Based on ASF, gas particles collide either with active or passive site
- Reactivity at active sites is much higher than at passive sites, and the reaction rate for oxidation (CO formation)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





Active Site Implementation in SPARTA





taken from [7]

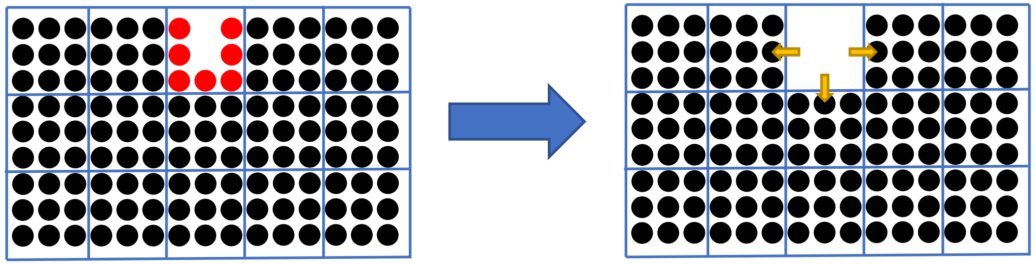
Algorithm:

- 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 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.

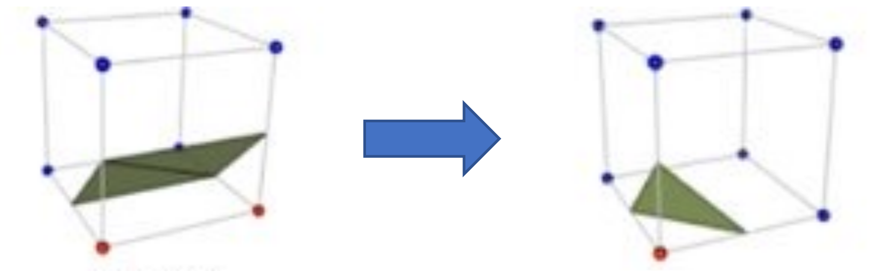
[7] Simon Schmitt *(2020), PhD thesis.*

Active Site Implementation in SPARTA



Algorithm:

- 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 [10]

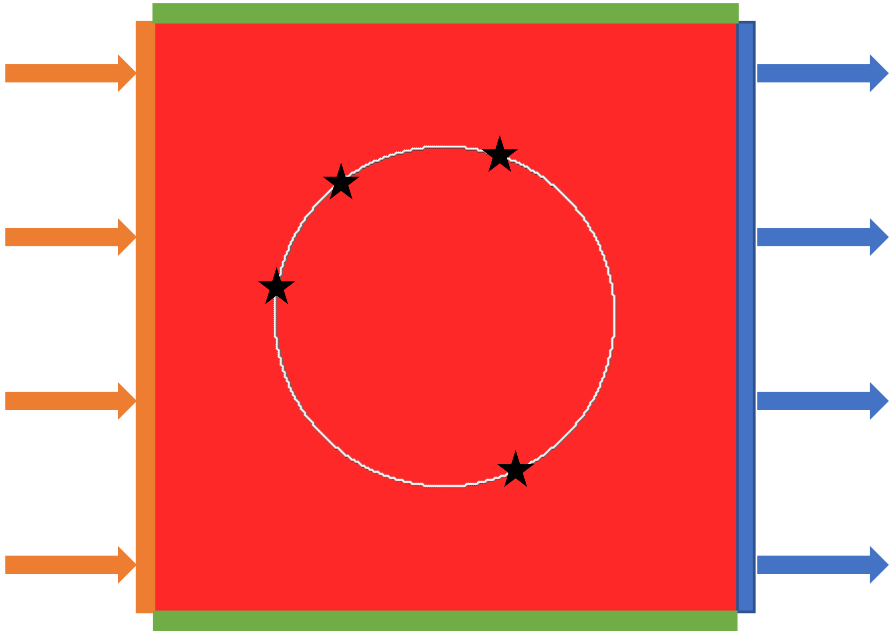
- Continuation through ablate step in DSMC
  - ❖ Before ablate – ASF of surface elements within a cell is averaged.
  - ❖ After ablate – ASF of new surface elements is set to this averaged value.

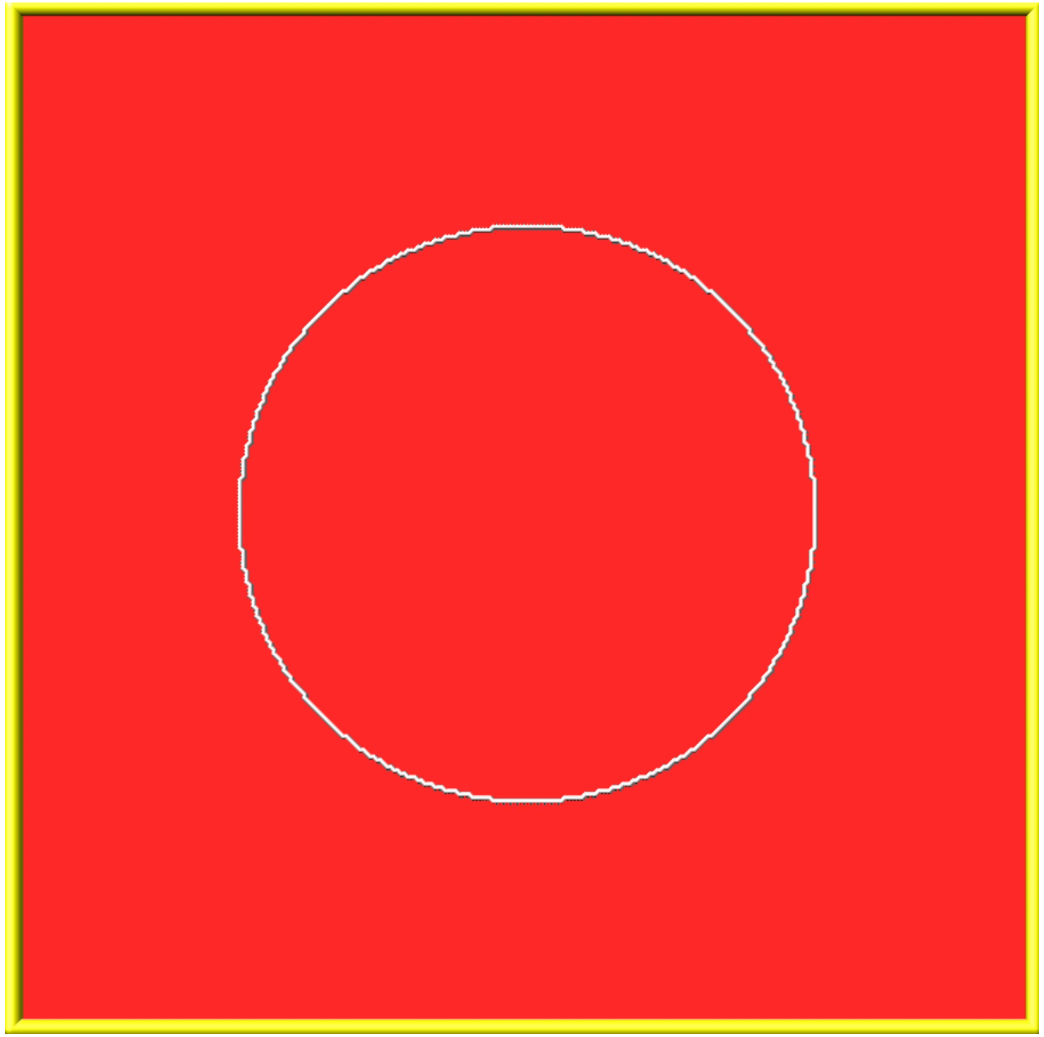
[10] Custodio et. al, An extended triangulation to the Marching Cubes 33 algorithm. J. Braz. Comp. Soc. (2019)

DSMC Results – 2D

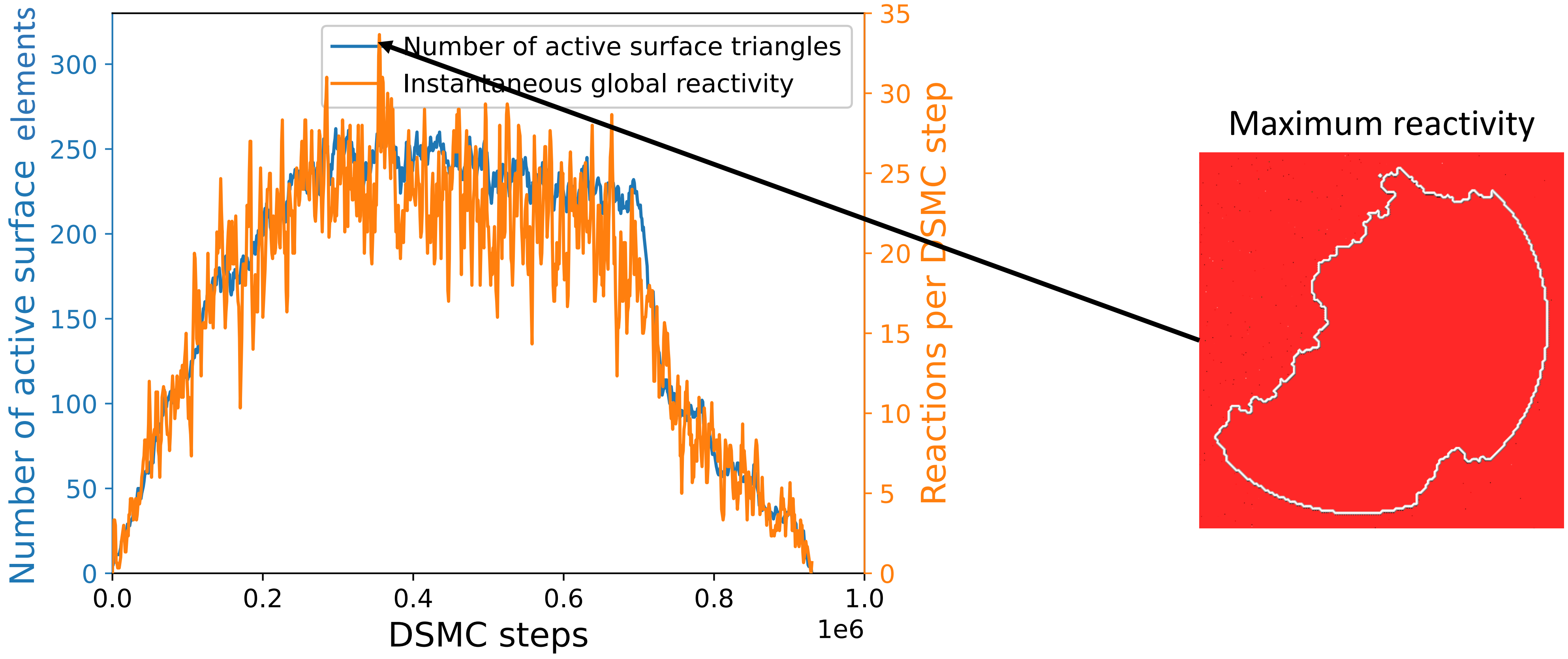
Simulation setup:

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



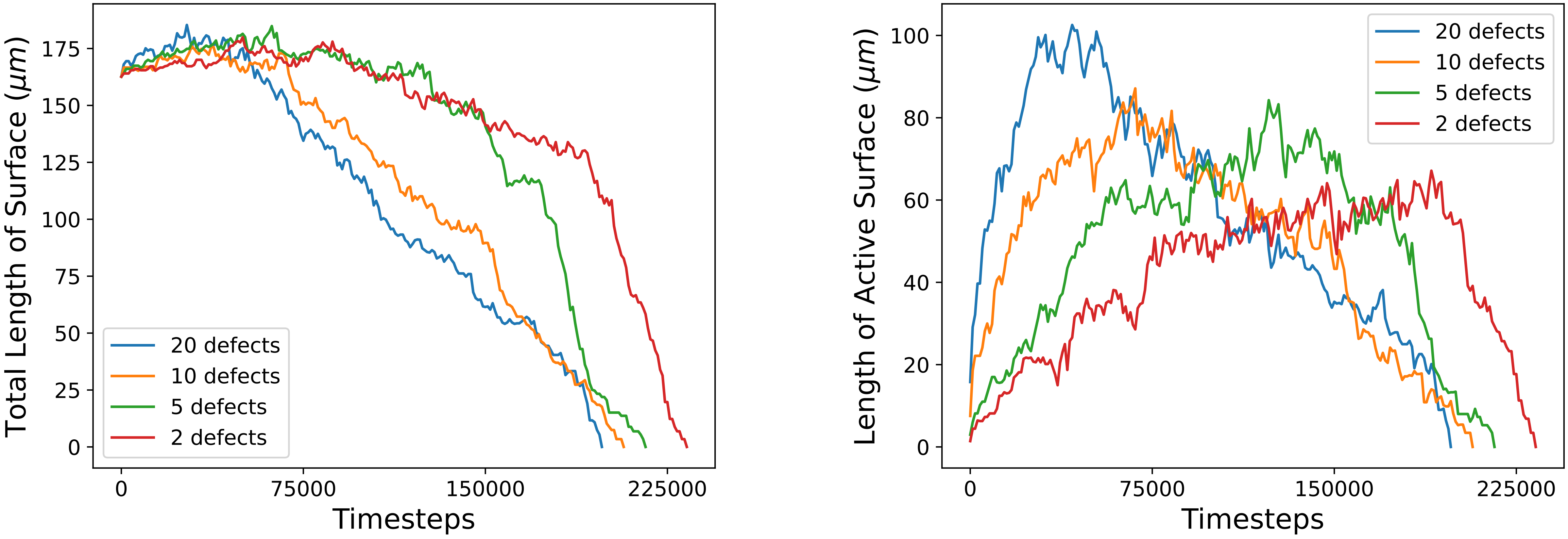


Evolution of active surfaces vs reactions



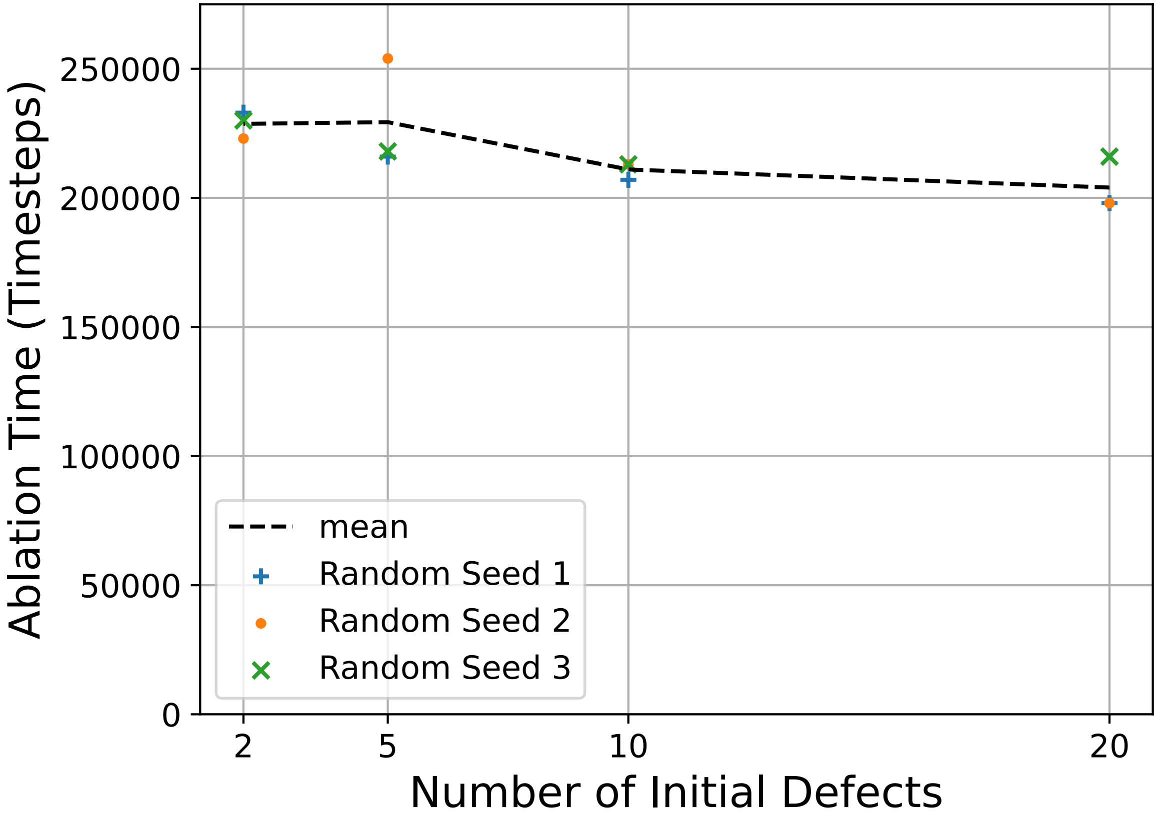
- Pitting causes nonlinear variation in reactivity due to active site evolution and flow-geometry interactions

Effect of defect density



- Total surface length initially increases with material removal.
- Peak in reactivity occurs earlier with increasing number of defects.

Total ablation time

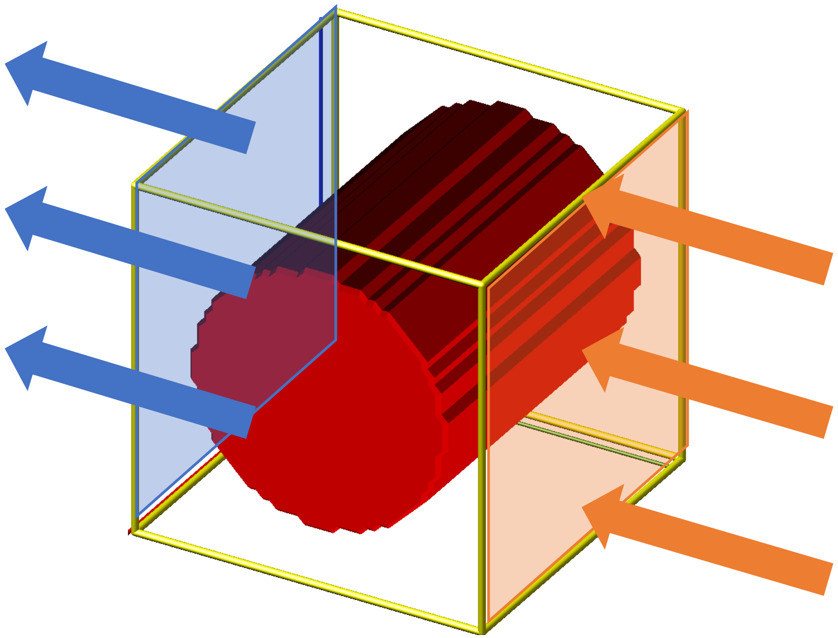


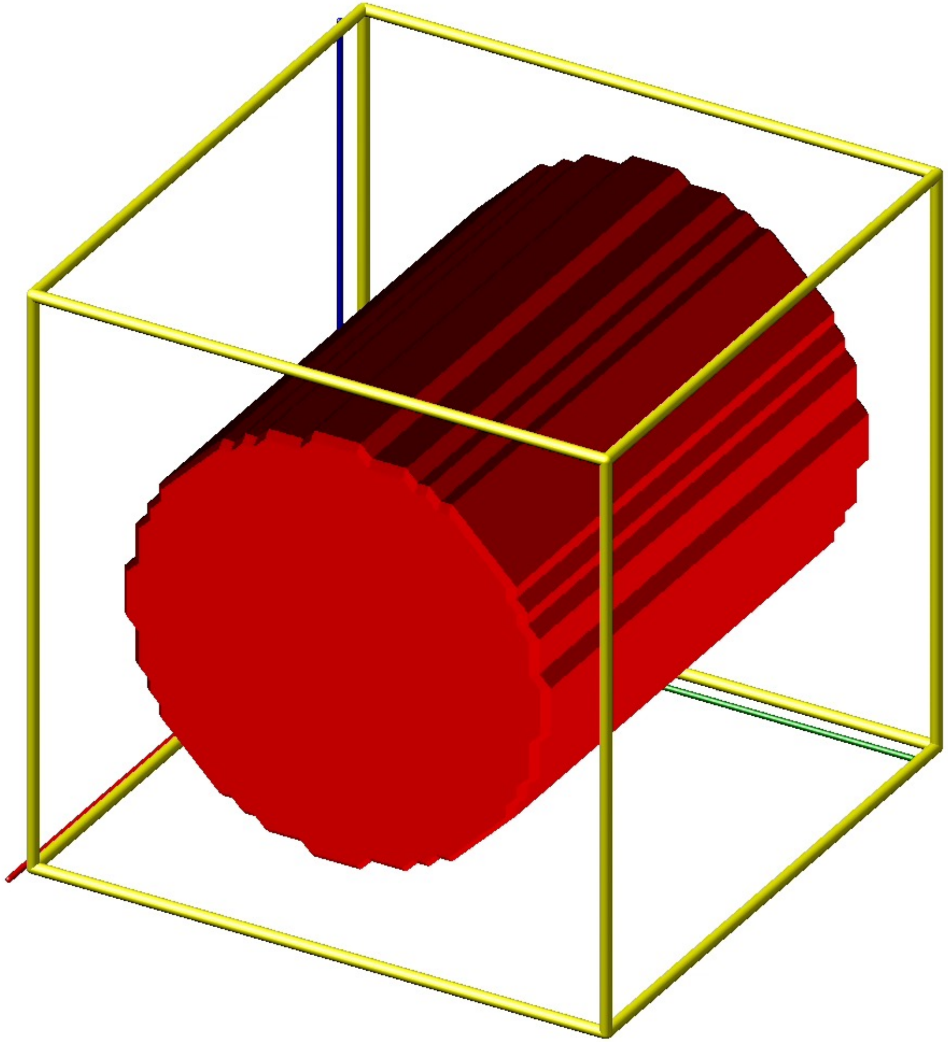
- Total ablation time decreases with increasing number of defects.
- Reactivity decreases after the peak due to decreasing surface area, leading to the ablation times being significantly closer.

DSMC Results – 3D

Simulation setup:

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



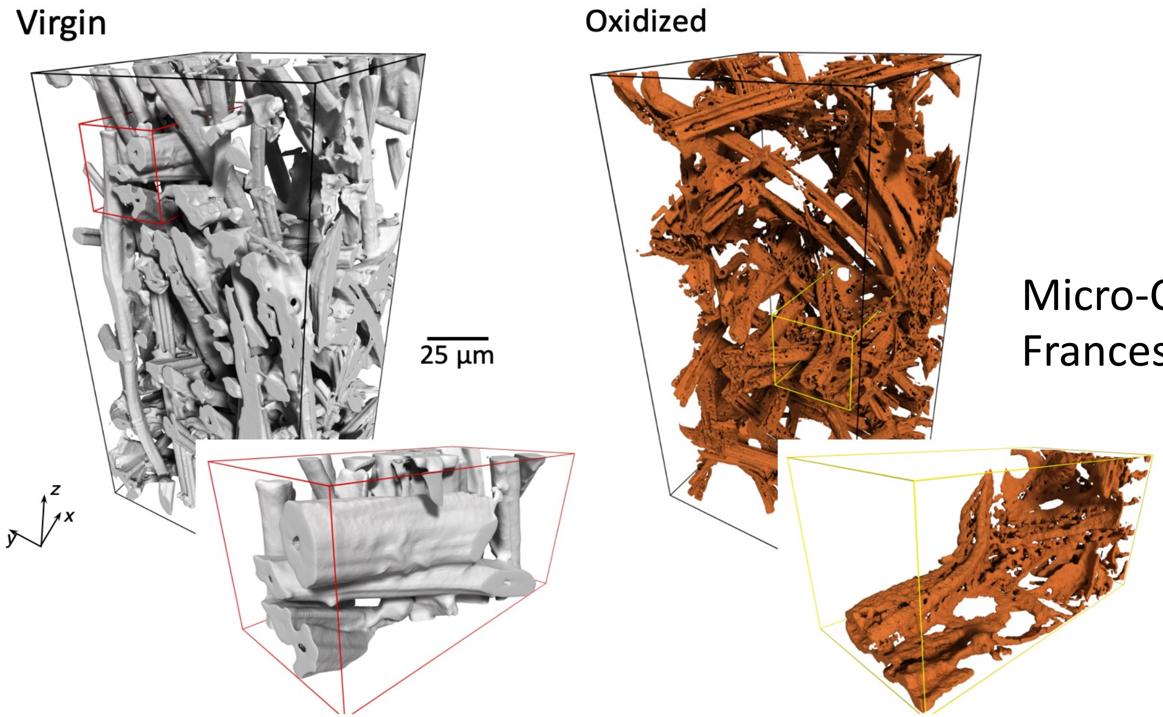


Summary

- Active-site-fraction feature was implemented in DSMC code SPARTA.
- Preliminary simulations of pitting resulting from active sites were performed.
  - ❖ Reactivity is directly linked to the active surface elements.
  - ❖ Pitting causes nonlinear variation in reactivity due to active site evolution and flow-geometry interactions.
- Effect of the number of defects was also investigated.
  - ❖ Peak in reactivity occurs earlier with increasing number of defects.
  - ❖ Total ablation time decreases with increasing number of defects.
  - ❖ Reactivity decreases after the peak due to decreasing surface area, leading to the ablation times being significantly closer.

Future Work

- Improve active-site feature in SPARTA to be more physically realistic.
- Extend SPARTA simulations to FiberForm
- 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

Questions?

National Aeronautics and Space Administration

Ames Research Center
Entry Systems and Technology Division