Multiphysics Multiscale Simulation Platform for Damage, Environmental Degradation and Life Prediction of CMCs in Extreme Environments

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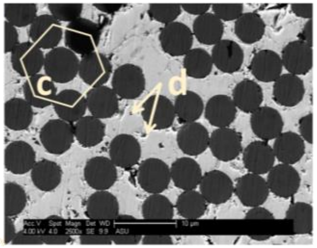
Overview

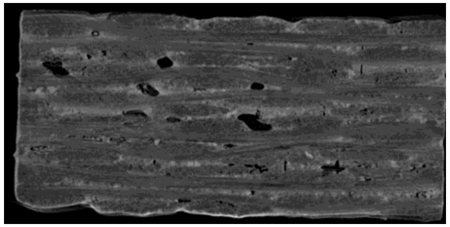
- **Objectives**
- **Project Summary**
- **Research Progress**
  - **Deep learning framework for automated microstructure characterization & reconstruction**
  - **Thermomechanical tests for S200H SiC/SiNC**
  - **Physics-based high-fidelity generalized method of cells microscale simulations**
  - **Neural network-based reduced order model formulations**
- **Concluding Remarks & Future Work**

Objectives

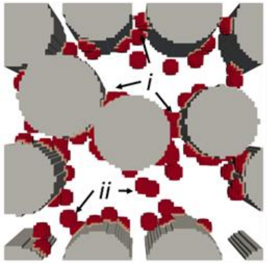
Develop a computationally efficient synergistic multiscale framework integrating multiphysics constitutive models with scale-specific experiments for damage assessment & life estimation of CMCs in service environment

- **Accurate scale-dependent material characterization & uncertainty quantification**
- **Constitutive modeling of damage, inelasticity, and effects of environmental degradation**
- **Integration of developed models into commercial finite element (FE) software for CMC component analysis**
- **Closed-loop testing & validation for model calibration & validation**

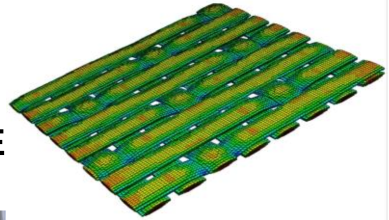




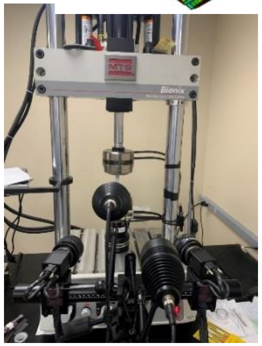
Micrographs



SRVE



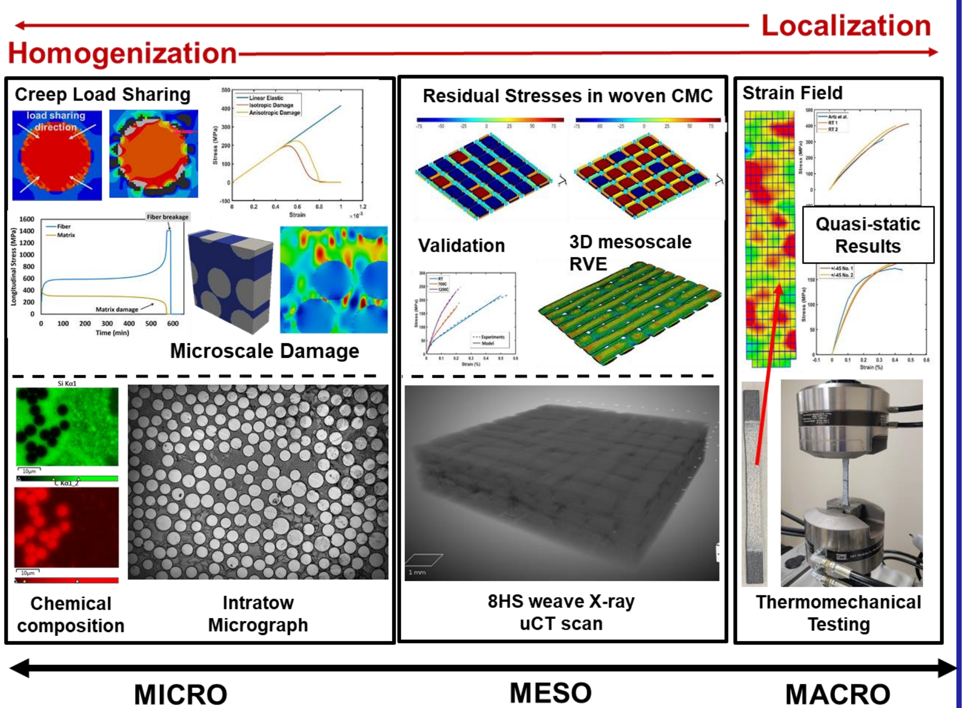
Thermomechanical testing



*Khafagy, K., Datta, S., & Chattopadhyay, A., *Journal of Composite Materials (2021)*

Project Summary

Methodologies



Multiscale framework integrating scale-specific multiphysics constitutive models with experimental characterization

Accomplishments

Previous year's work:

- **Scale-dependent variability characterization of C/SiNC and SiC/SiNC CMCs via microscopy & X-ray micro-computed tomography (uCT)**
- **Image processing algorithm for feature identification and generation of stochastic representative volume element (SRVE)**
- **Machine-learning (ML)-based techniques to facilitate image segmentation, scale-dependent variability quantification, and SRVE generation**
- **High fidelity damage modeling to investigate effects of microporosity and residual stress in SiC/SiC composites**
- **Quasi-static tensile testing of 8HS woven SiC/SiNC CMC with in-situ digital image correlation (DIC)**
- **Coupled oxidation and damage model**

Current work:

- **Creep-fatigue testing and microstructure assessment for woven SiC/SiNC and C/SiNC CMC**
- **ML-based SRVE generation and implementation for high fidelity models**
- **Physics-informed neural-network (NN)-based surrogate model to emulate multiscale methodology**

Milestone

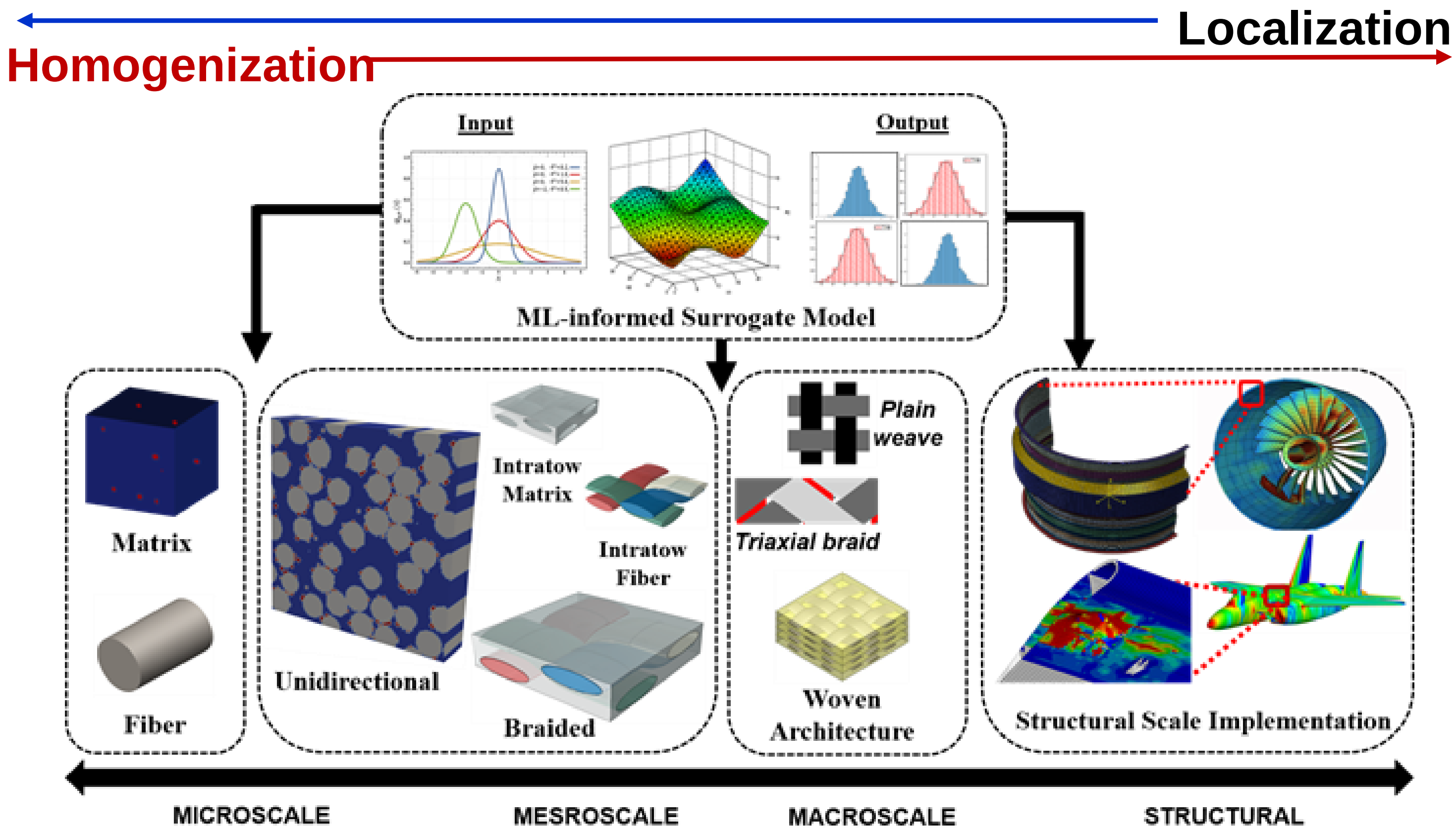
	BP1	BP2	BP3	BP4	BP5
	8/16/19 – 9/30/19	10/1/19 – 9/30/20	10/1/20 – 9/30/21	10/1/21 – 9/30/22	10/1/22 – 8/15/23
	Qtr1 Qtr2 Qtr3 Qtr4	Qtr1 Qtr2 Qtr3 Qtr4	Qtr1 Qtr2 Qtr3 Qtr4	Qtr1 Qtr2 Qtr3 Qtr4	Qtr1 Qtr2 Qtr3 Qtr4
Task 1: Project Management and Planning					
Task 2: Material Characterization and Uncertainty					
Task 3: Multiphysics Constitutive Modeling with Thermomechanical Damage					
Task 4: Integrated Multiscale Framework					
Task 5: Integration into FE Model					
Task 6: Closed Loop Testing and Validation					

Completed: Projected:

Research Team

- **Dr. Aditi Chattopadhyay – PI**
- **Dr. Luke Borkowski (RTRC)–Major Participant**
- **Mohamed Hamza – PhD Student**
- **Rayva Ranade – MSc Student**
- **Christopher Sorini – PhD Student/Dean's Scholar**
- **Khaled Khafagy – PhD Student**
- **Jacob Schichtel – NDSEG fellow, no cost to the grant**

Synergistic Multiscale Modeling Framework



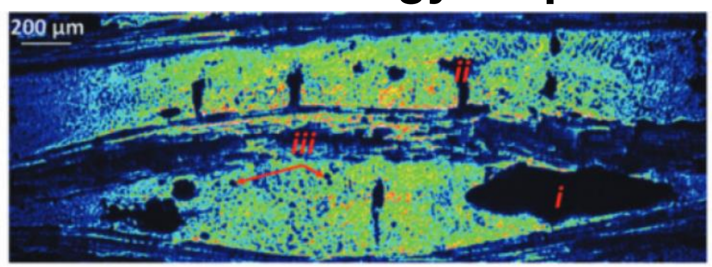
- Multiscale framework using multiscale generalized method of cells (MSGMC, Liu & Chattopadhyay, 2011) - generalizes two-scale homogenization & localization operations to arbitrary number of scales
- Allows synergistic analysis of woven or braided composite systems
- Model damage & inelasticity at constituent level & capture progression to higher length scales
- Reduced order models for computational efficiency

Scale-dependent Variability

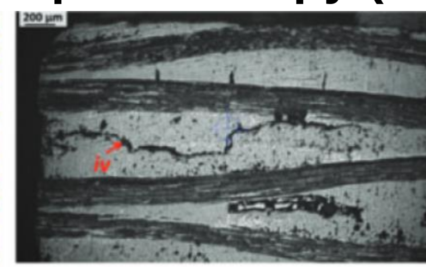
Multiscale material & scale-dependent architectural variability quantification: i) extract scale-dependent architectural features & defect variability from micrographs; ii) construct statistical representative volume elements (SRVEs) inform multiscale modeling framework

- **Meso/macroscale - X-ray micro-computed tomography (uCT)**
- **Microscale - confocal microscopy (CM) & scanning electron microscopy (SEM)**
- **Chemical elemental characterization - energy dispersive spectroscopy (EDS)**
  - Mesoscale
    - Inter-tow defects;
    - tow size & shape
    - Inter-tow spacing
  - Microscale
    - Intra-tow fiber vol. %
    - Fiber radii & spacing
    - Intra-tow porosity vol. %

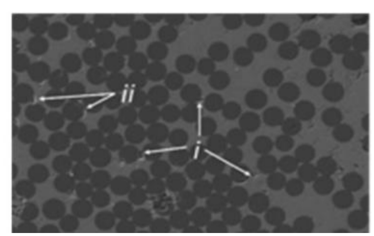
Previously - semantic segmentation algorithm using deep learning based framework

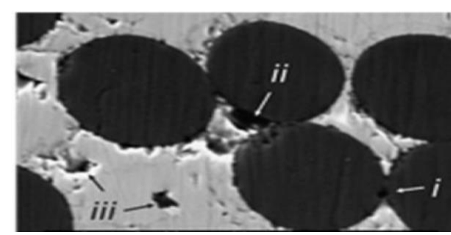


Denuded matrix defects: Open and intra-tow porosity



Crack nucleation at free surface





CMC intra-tow porosity

Khafagy, K., Datta, S., & Chattopadhyay, A., *Journal of Composite Materials (2021)*

Automated Microstructure Characterization & Generation

Deep learning (DL) framework: i) Deep Convolutional Nonlinear Regression for automated feature extraction; ii) Deep Conditional Generative Adversarial Network for SRVE generation

Challenges:

- Unified feature extraction & regression models
- Random generation of synthetic microstructure
- Coupling between variability & generated RVEs – *generate microstructures based on desired microstructure* variability
- Sparsity in micrographs

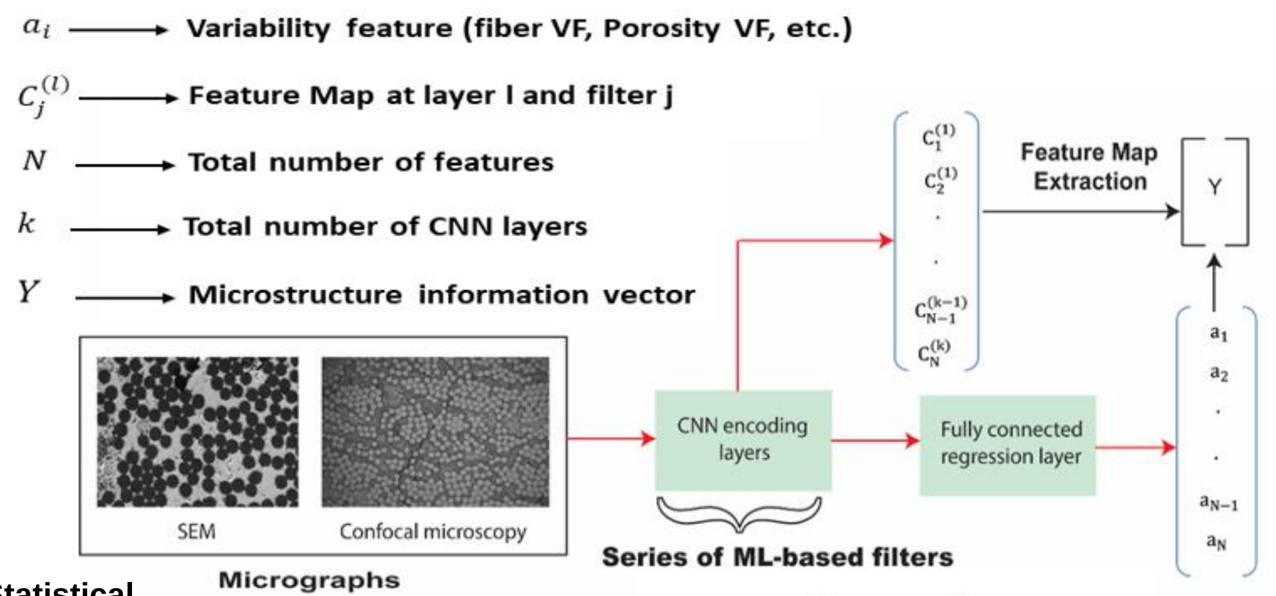
Advantages

- **Semantic segmentation of microstructure characteristic features through CNN layers**
- **Variability quantification through fully connected regression layers**
- **Vanilla regression output tensor used to train generative adversarial network (GAN)**
- **Various GAN architectures used for high-fidelity microstructure reconstruction**
- **Microstructure-inspired statistically representative volume elements (SRVEs)**
- **Applicable to other material systems with complex heterogeneous architectures**

Automated Microstructure Characterization & Generation

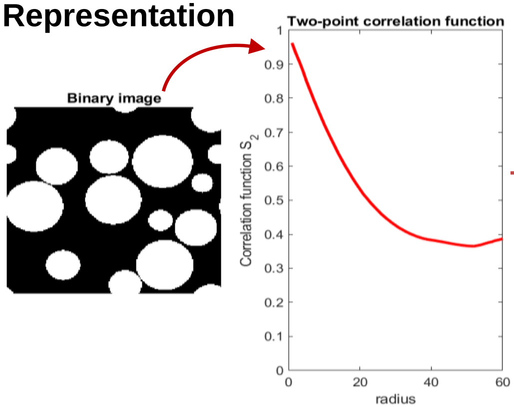
Vanilla Regression NN for CMC Characterization

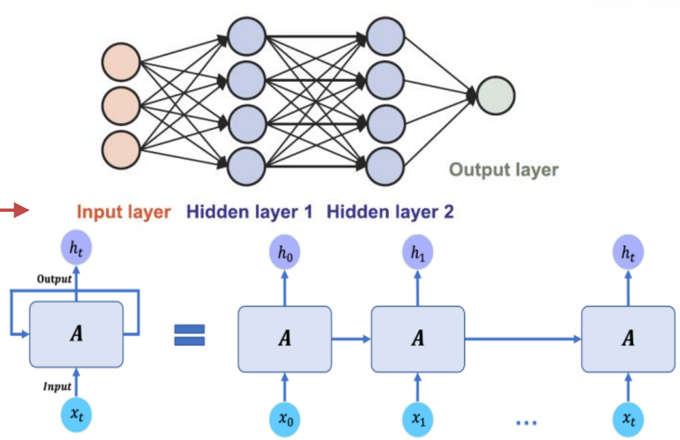
Spans taxonomy of microstructure analysis: semantic segmentation of microstructure constituents & quantification of microstructure variability



Statistical Descriptors:
- Two-point correlation

Statistical Representation

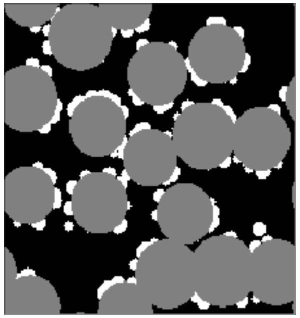




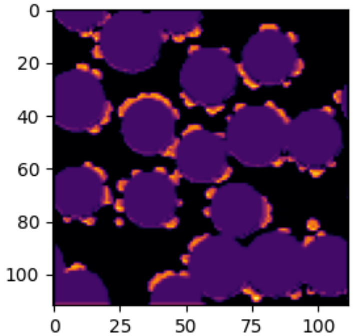
Physical Descriptors
- Fiber volume fraction
- Mean fiber radius
- Porosity fraction

Vanilla Regression Training

Used previously-developed computer vision (CV) SRVE generation algorithm to train DL-based algorithm & further improve variability quantification accuracy

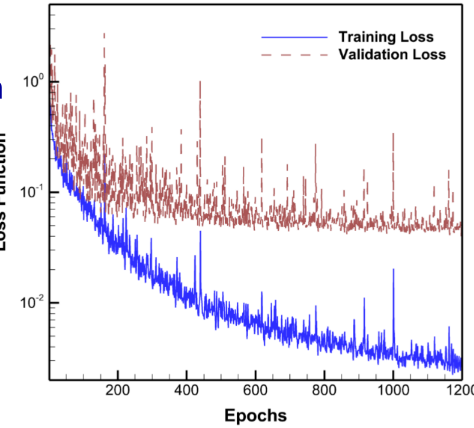


Computer-vision training microstructure



Deep-learning Segmented microstructure

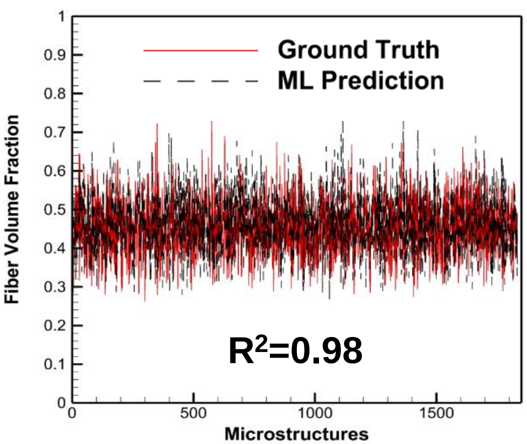
Loss function Minimization

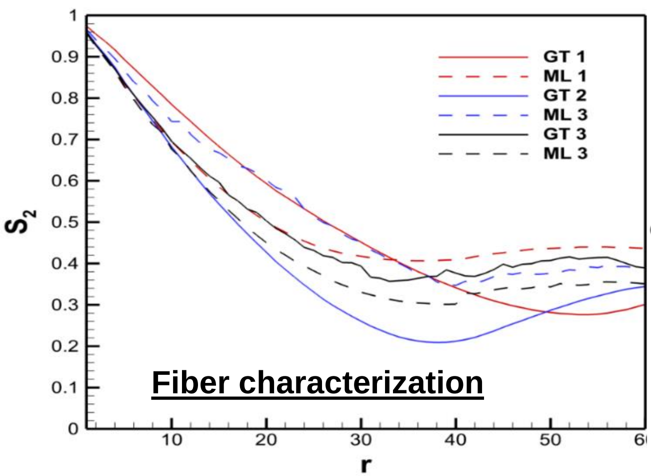


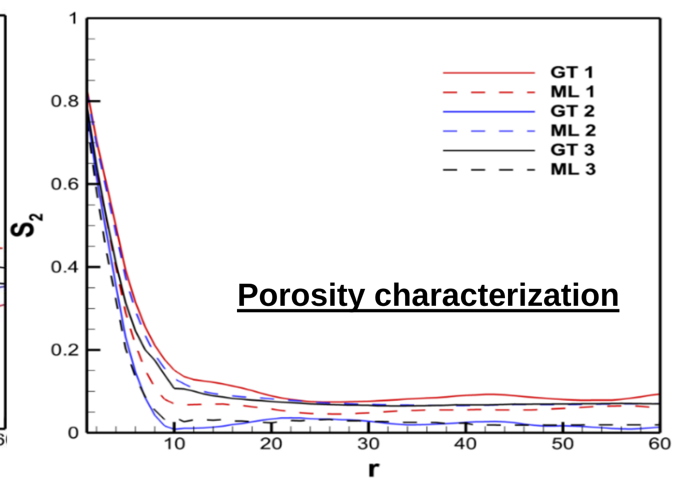
Two-point Correlation

$$s_2^i(r) = < I_p(x), I_p(x+r) >$$

$$I_P(z) = \begin{cases} 1 \; if \; z \in phase \; i \\ 0 \; otherwise \end{cases}$$

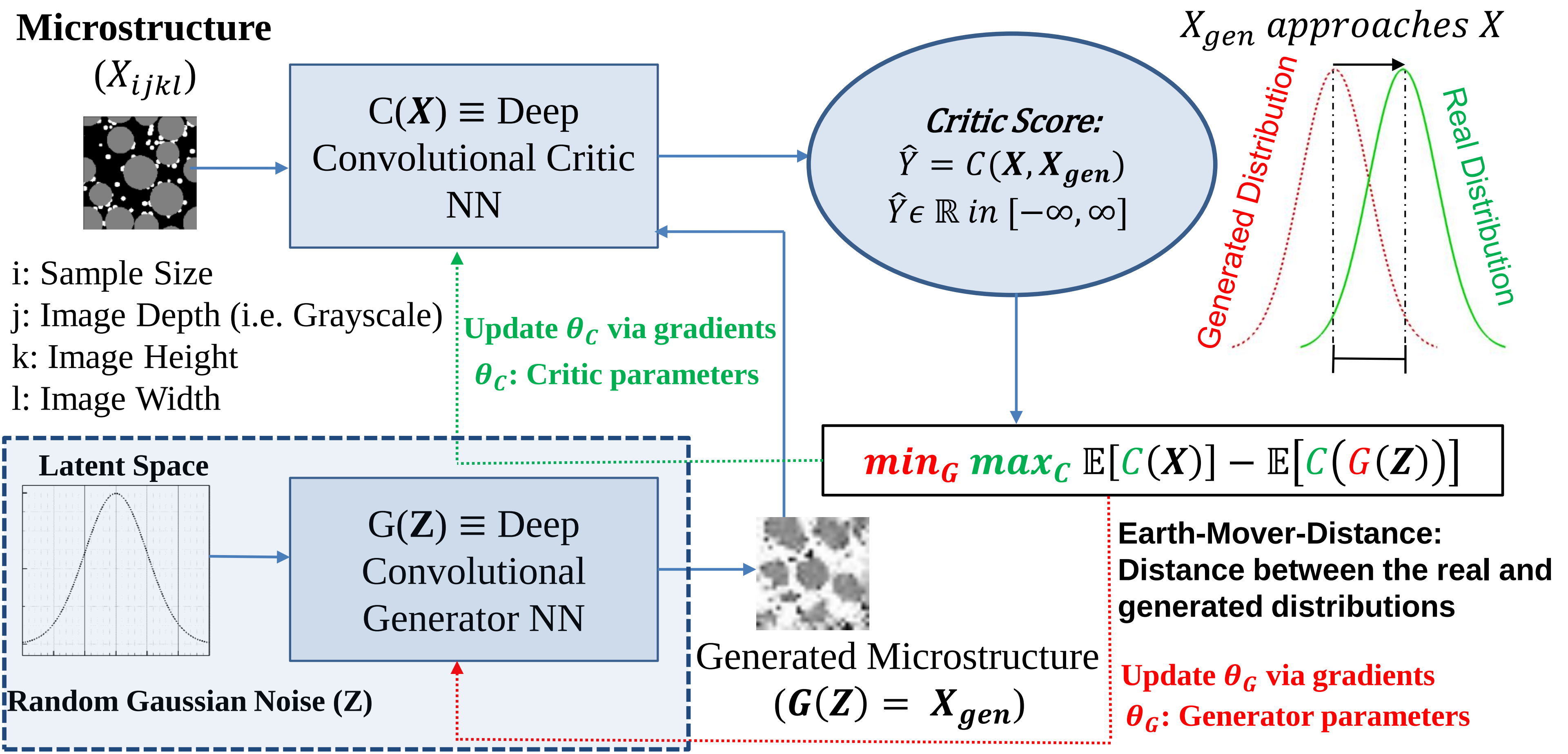






- Optimized vanilla regression variability prediction show high coefficient of determination (R^2) with respect to the ground truth
- Deep vanilla regression captured fiber and porosity radial correlation functions overall trend

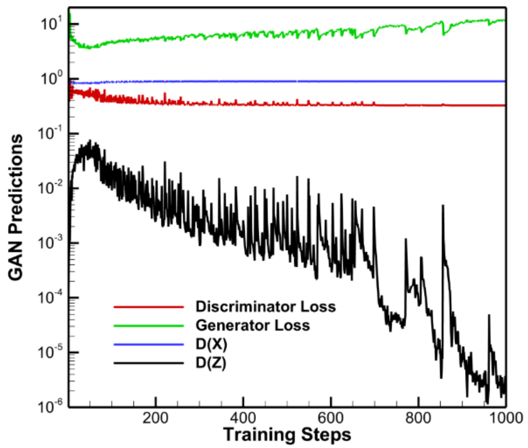
Multi Deep NN for CMC SRVE Generation

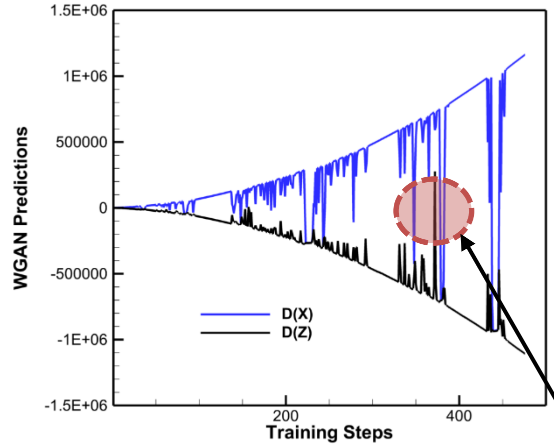


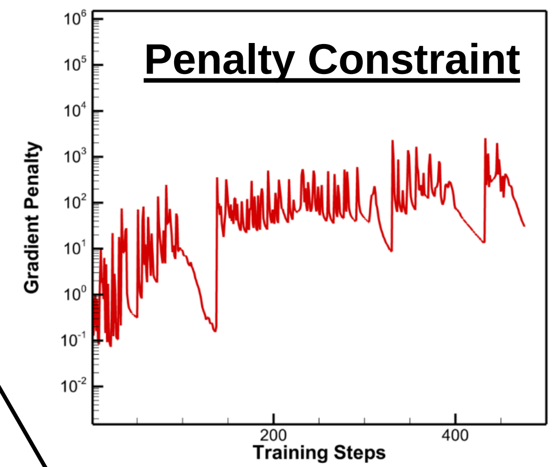
Wasserstein Generative Adversarial Network (WGAN) Outcomes:

- **Critic network learns microstructure convolution filters to distinguish between actual micrographs and generated SRVEs by maximizing the Wasserstein loss**
- **Generator network produces SRVEs which mimic the actual micrographs, thus minimizing the Earth-Mover-Distance (EMD) between the two distributions**

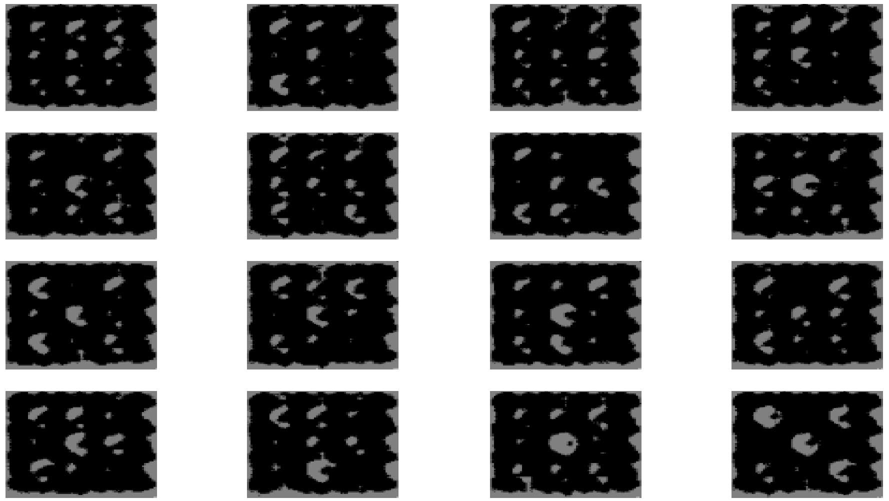
SRVE Generation and Training Evaluation



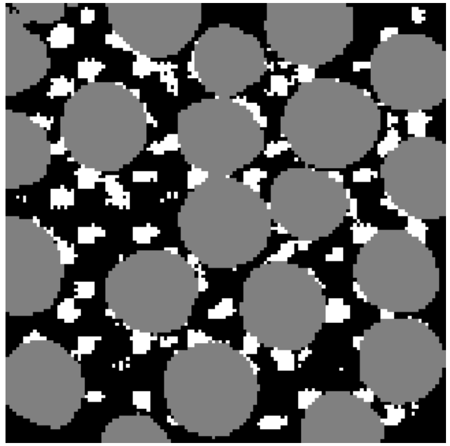




SRVE Evolution Across Model Training

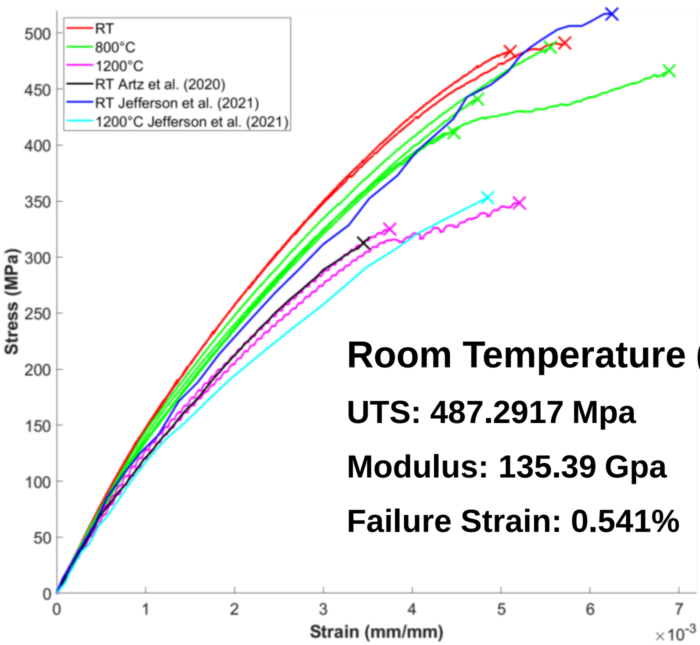


Optimized Generated SRVE



WGAN showed enhanced SRVE quality generation with microstructure variability compared to traditional GAN frameworks due to better gradient estimations and stable objective function

S200H SiC/SiNC Quasi-Static Tests



Room Temperature (RT)

UTS: 487.2917 Mpa

Modulus: 135.39 Gpa

Failure Strain: 0.541%

800ºC

UTS: 451.2897 Mpa

Modulus: 128.47 Gpa

Failure Strain: 0.541%

1200ºC

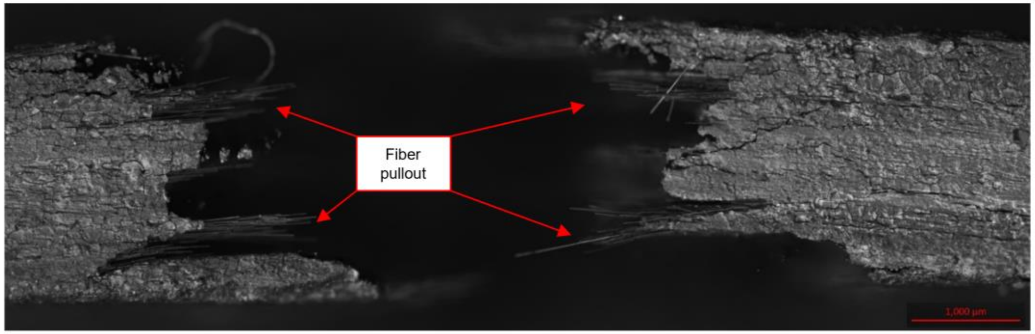
UTS: 336.5265 Mpa

Modulus: 110.83 GPa

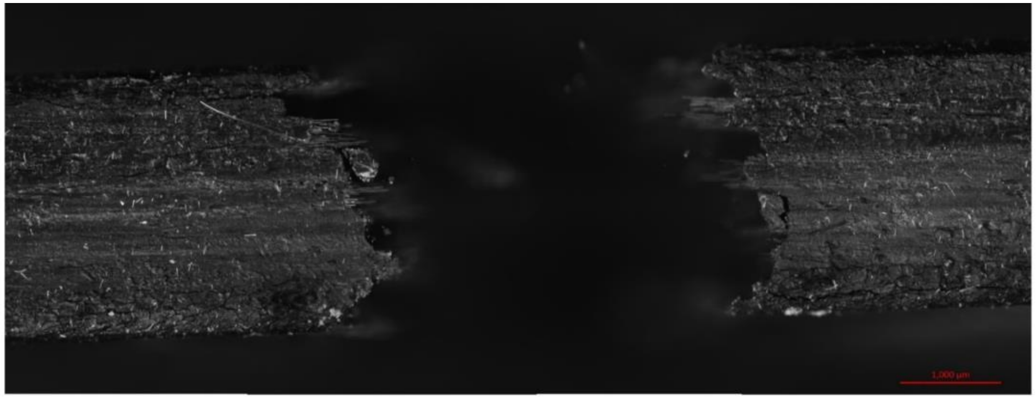
Failure Strain: 0.448%

Confocal Micrographs of Fracture Surface

RT

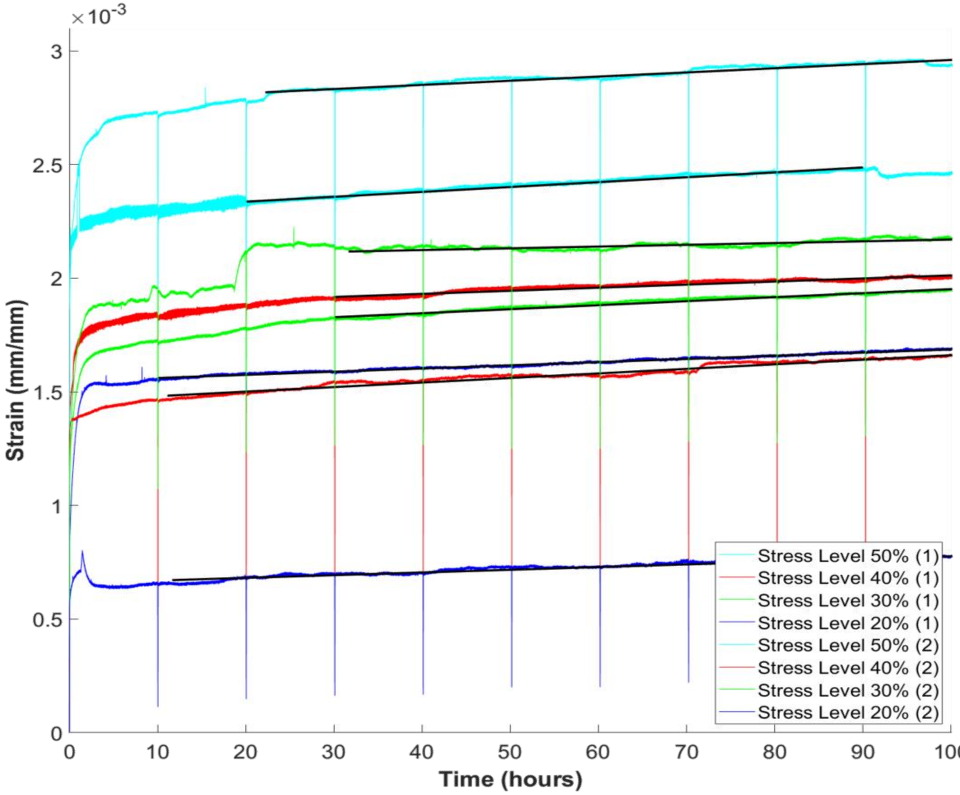


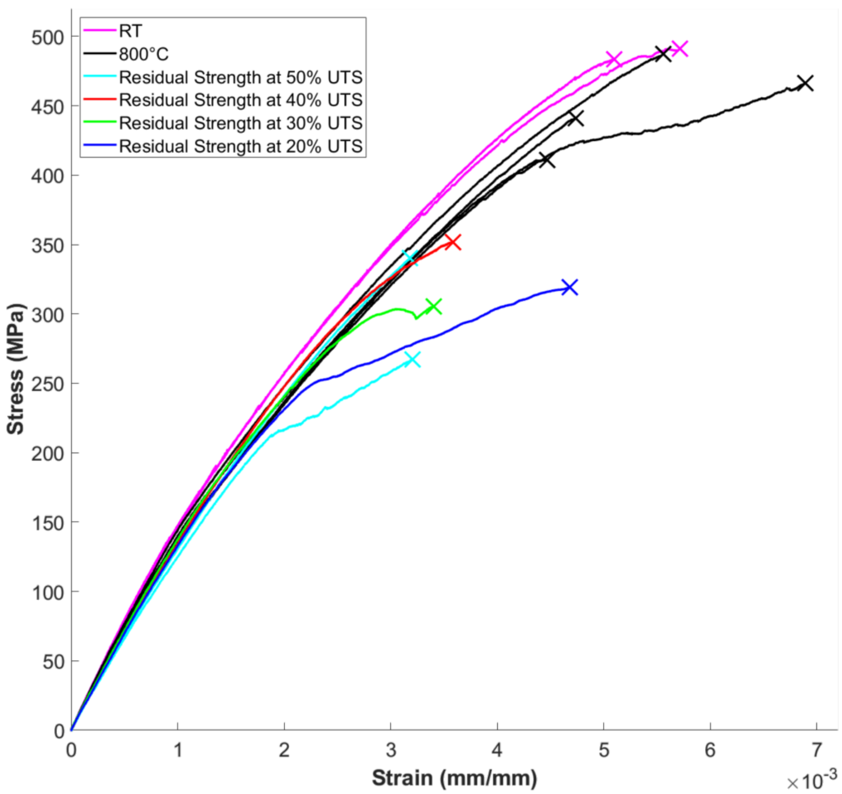
800ºC



- **Nonlinear behavior is due to large pores and cracks caused by PIP manufacturing process; accelerating damage growth in the composite**
- **Tensile strength results at 1200ºC are in good agreement with literature**
- **Drastic decrease in tensile strength at 1200ºC due to higher activation energy for matrix microcracks**

S200H SiC/SiNC Creep-Fatigue and Residual Strength Tests

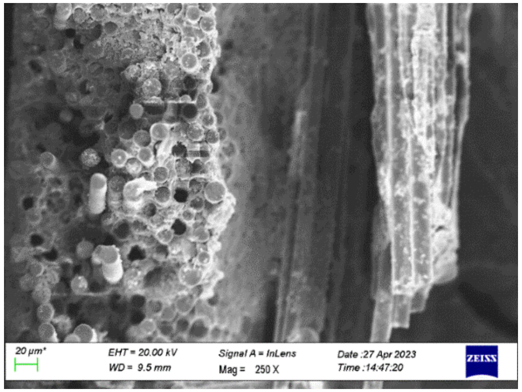




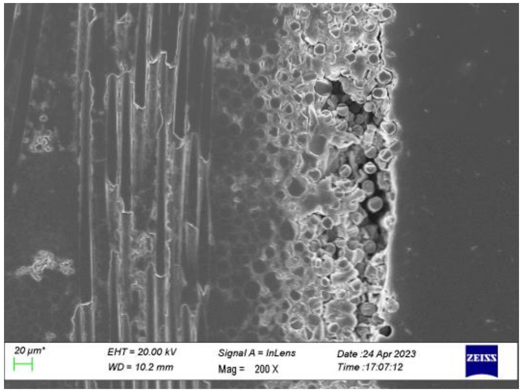
- **Large difference in strain between repeated tests at 50% and 40% Stress Levels**
- **Strain rates for repeated tests at 50%, 40% and 30% stress levels match**
- **Stiffness decreased due to embrittlement caused by oxidation**
- **Significant decrease in strength and strain to failure upon creep-fatigue exposure**

S200H SiC/SiNC Fracture Post-Residual Strength (800ºC)

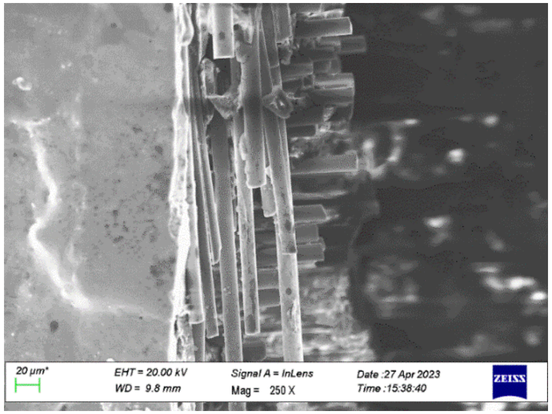
Cross section of fracture surface



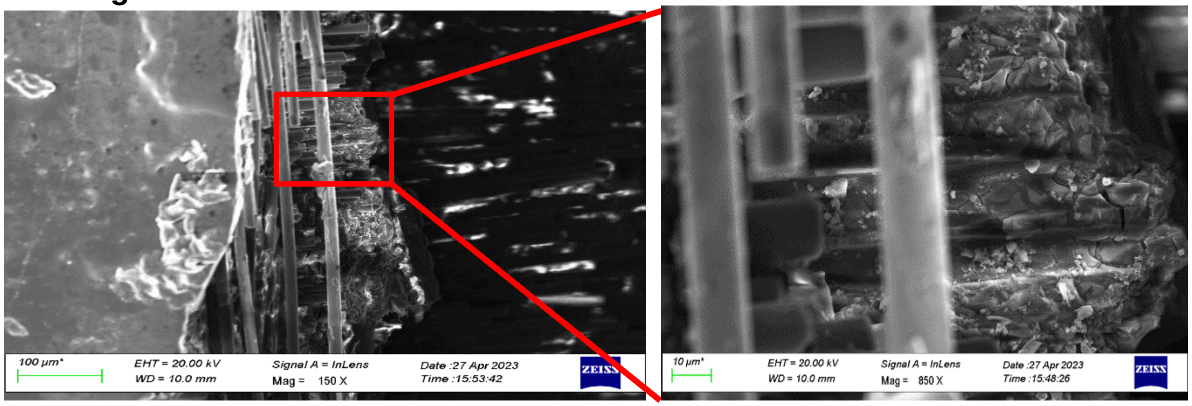
Manufacturing-induced damage on fracture surface



Void in matrix leaving exposed fibers



Fracture damage located close to sample surface



Silica formation on fracture surface

- Material characterization using SEM and EDS performed after creep-fatigue testing and residual strength testing
- Damage due to manufacturing induced defects depicted in sample fracture surface
- SiNC matrix oxidizes into glassy silica phase causing embrittlement

Physics-based High-fidelity Modeling of CMCs

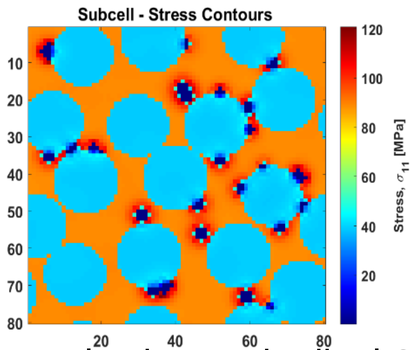
Key Features

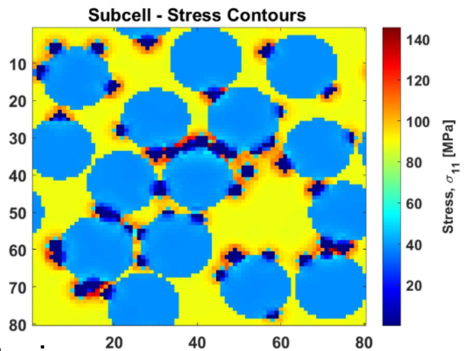
- Modeling CMC viscoplasticity and damage induced inelasticity at elevated temperature
- Capturing the CMCs global mechanical response due to damage mechanisms in each constituents (fiber and matrix)
- Model training on high-fidelity microstructure representation to account for microstructure features and variability effects
  - Capturing the main stages of creep strain behavior
  - Enforcing physics-based constrains through loss function regularization
  - Microscale surrogate model training on stress relaxation and creep testing scenarios with damage

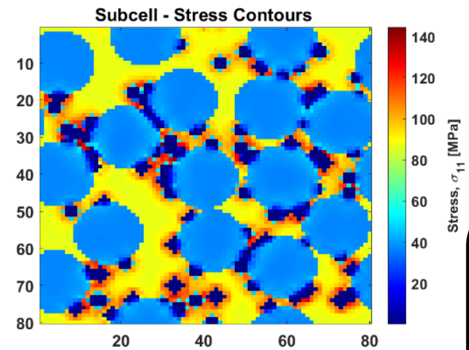
Stress Relaxation for S200H CMC at 1300ºC: Localized Response

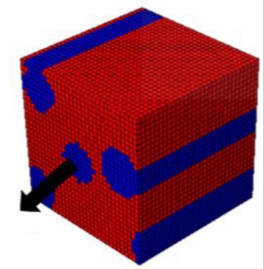
1% defect VF	2% defect VF	4% defect VF	Applied Strain

Cauchy Longitudinal Stress:

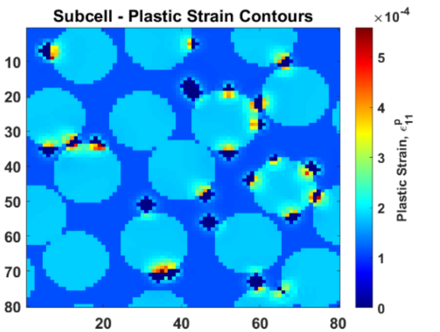


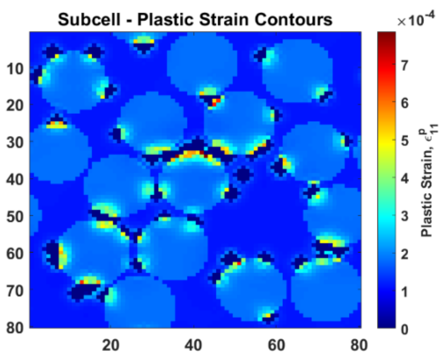


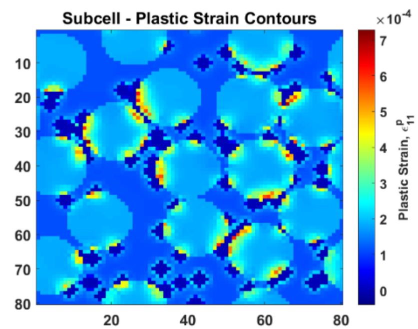




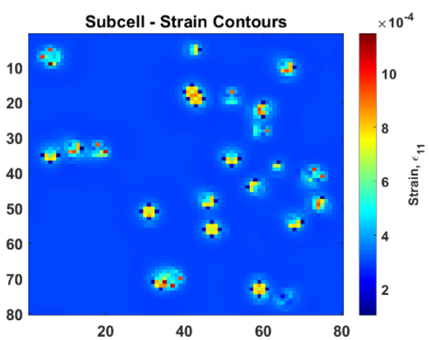
Inelastic Longitudinal Strain:

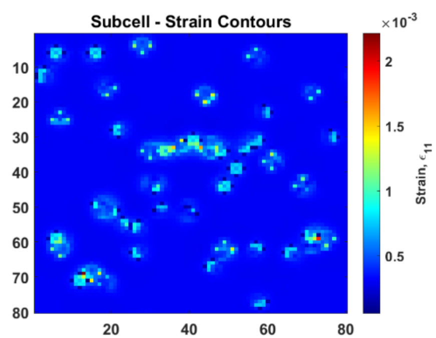


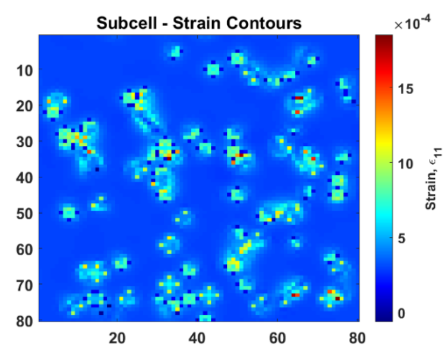




Total Longitudinal Strain:

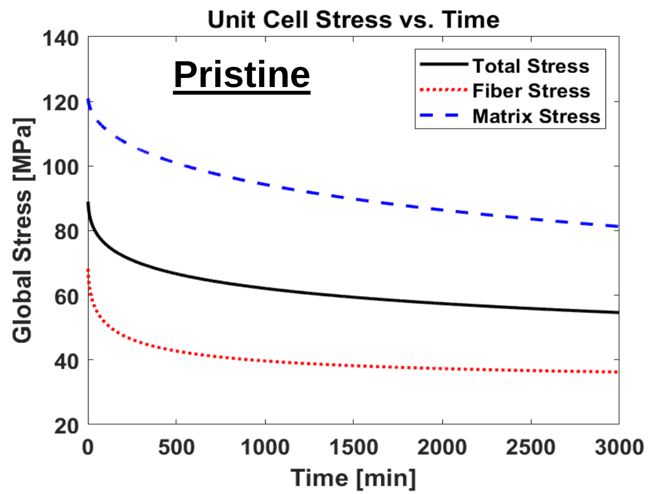


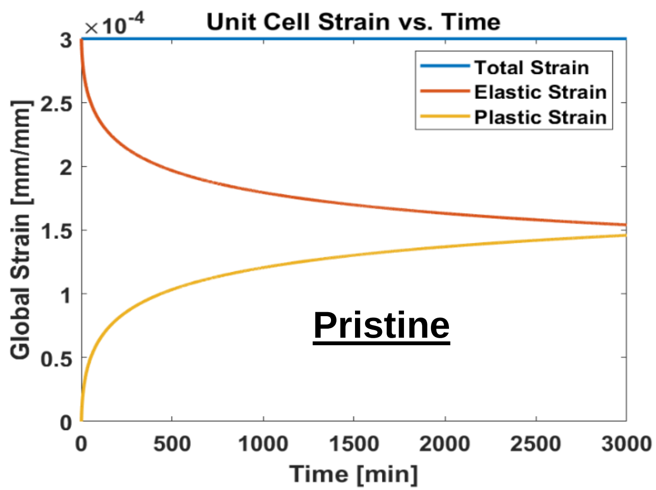


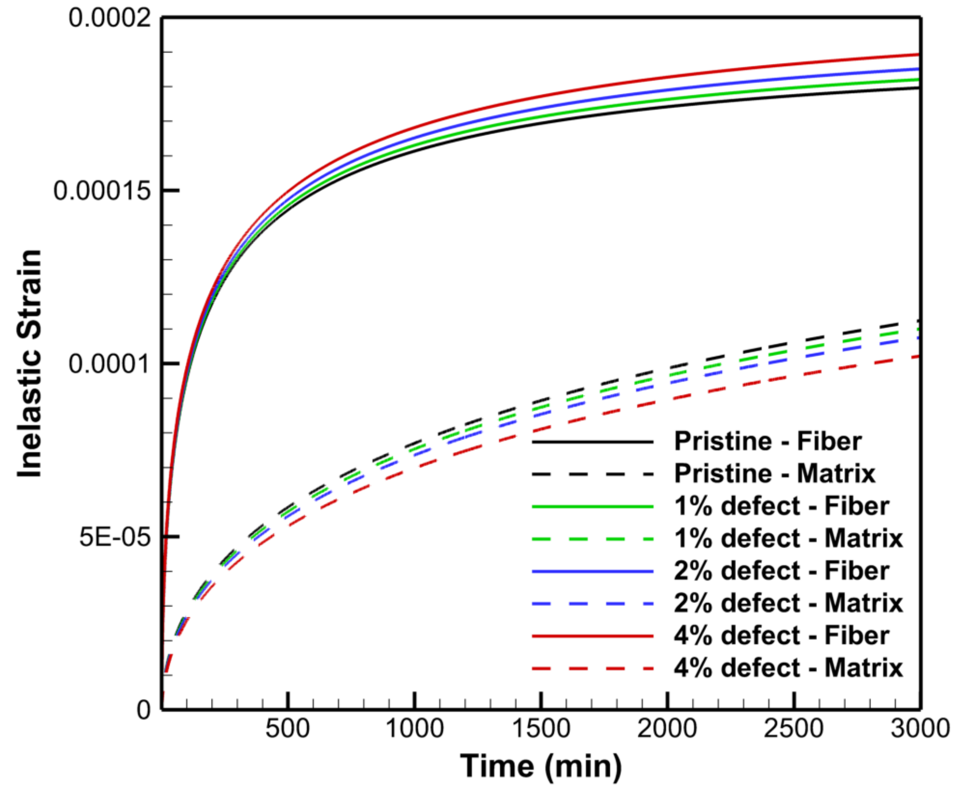


- **Intratow defects induced localized stress and viscoplastic strain around fiber surfaces**
- **Viscoplastic strain mismatch between SiNC matrix and Hi-Nicalon fiber due to different stress state and inelasticity activation energy**
- **Localized total strain near porosity; indicating defects diffusion along fiber surfaces during stress relaxation**

Impact of Porosity on Inelastic Response of S200H CMC at 1300ºC





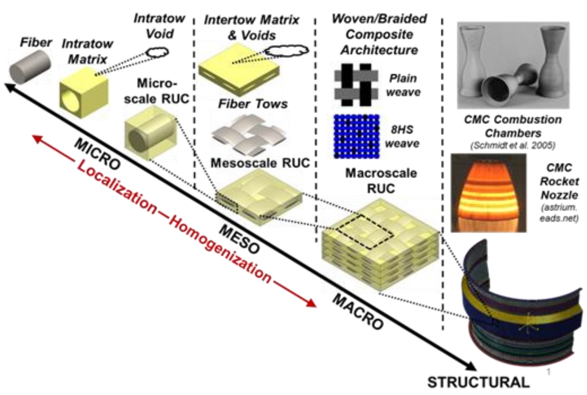


- **S200H exhibits inelastic strain mismatch during stress relaxation simulations**
- **Fiber stress rapidly drops and approaches a constant creep strain rate**
- **Inelastic strain in fiber increases with porosity as a result of stress localization along fiber surfaces**

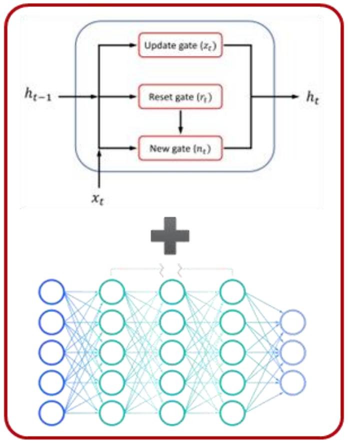
Physics-Informed Machine Learning CMC Surrogate Model

Surrogate model developed and extended to effectively predict response of woven SiC/SiC with microstructural variability

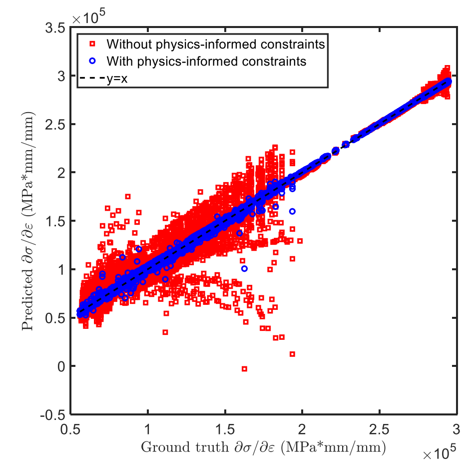
Multiscale model for training ML surrogate model



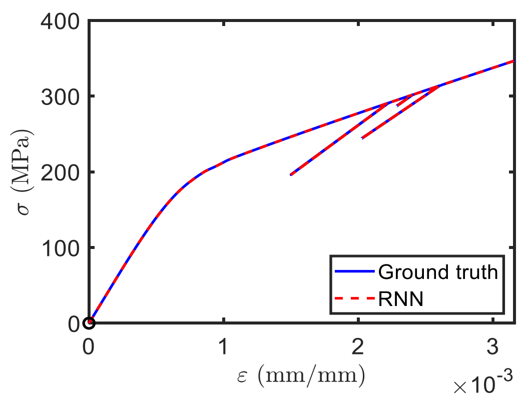
RNN-based, physics-informed surrogate model



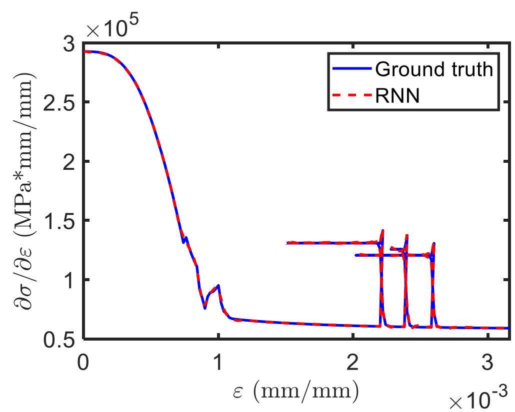
Parity plot – with and without physics-informed constraints



Stress vs. strain



Tangent modulus vs. strain



Prediction speedup

Model	Runtime (s)	Speedup (times)
Numerical	116.41	NA
Surrogate (CPU)	2.22e-3	5.2e4
Surrogate (GPU)	2.08e-4	5.6e5

*Borkowski, L., Skinner, T., & Chattopadhyay, A. (2023). Woven ceramic matrix composite surrogate model based on physics-informed recurrent neural network. *Composite Structures*.

Concluding Remarks

- Variability quantification and generation of microstructure morphology
  - Deep learning (DL) model for microstructure features quantification
  - Microstructure-inspired representative volume element generation for microscale constitutive modeling

- Thermomechanical testing: Quasistatic high temperature and creep-fatigue
  - S200H SiC/SiNC showed significant nonlinearity due to porosity and shrinkage crack induced through manufacturing PIP process
  - Matrix microcracking and fiber brittle fracture control SiC/SiNC failure at elevated temperatures
  - Silica formation observed in SiNC matrix above 800^{o}C

- High-fidelity generalized methods of cells captured viscoplastic and damage mechanisms at the intratow level
  - Analyzed the impact of S200H CMC defects on stress relaxation and localized inelastic response

Future Work

- Computationally efficient deep learning-based surrogate modeling training based on high-fidelity simulations
- Dwell-fatigue modeling through coupling damage, viscoplastic creep and oxidation models
- Extension of oxidation model to include matrix reactions, fusing, crack sealing & refine formulation for enforcing surface-based reactions
- Fracture mechanics-based damage model development with temperature effects to capture matrix microcracking activation at elevated temperatures

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Jacob Schichtel – PhD (Mechanical Core Competency, Intel, Chandler)
Christopher Sorini – PhD (SWRI)

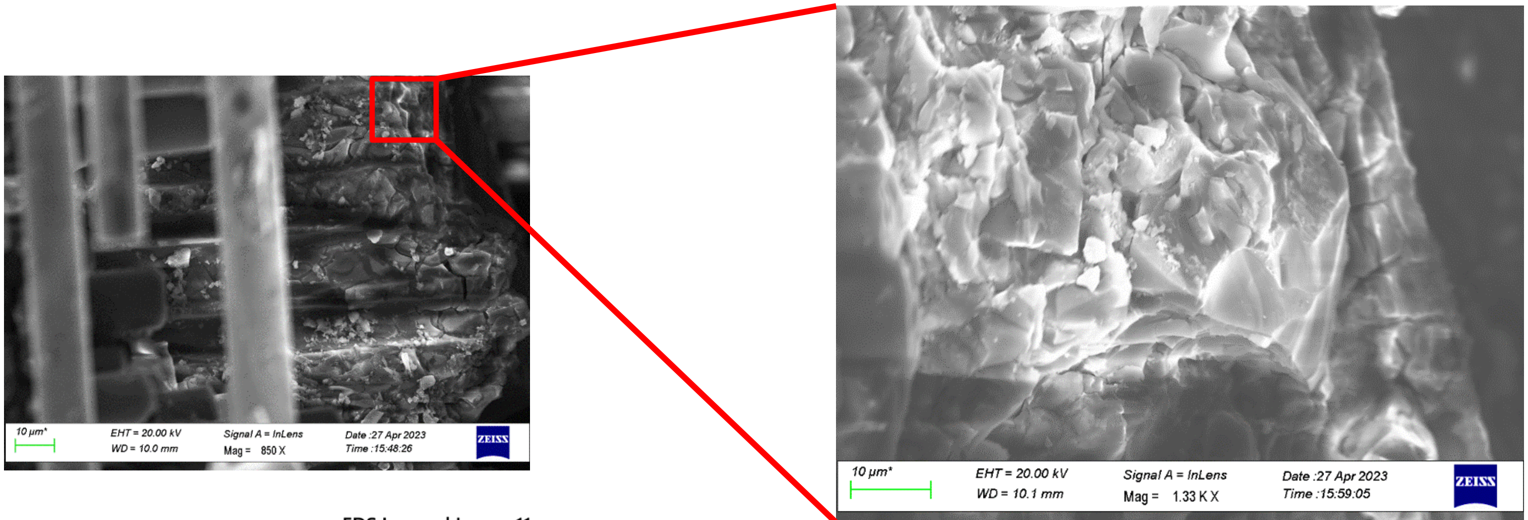
Backup Slides

Test Setup for Intermediate Temperature Quasi-Static Tensile Test

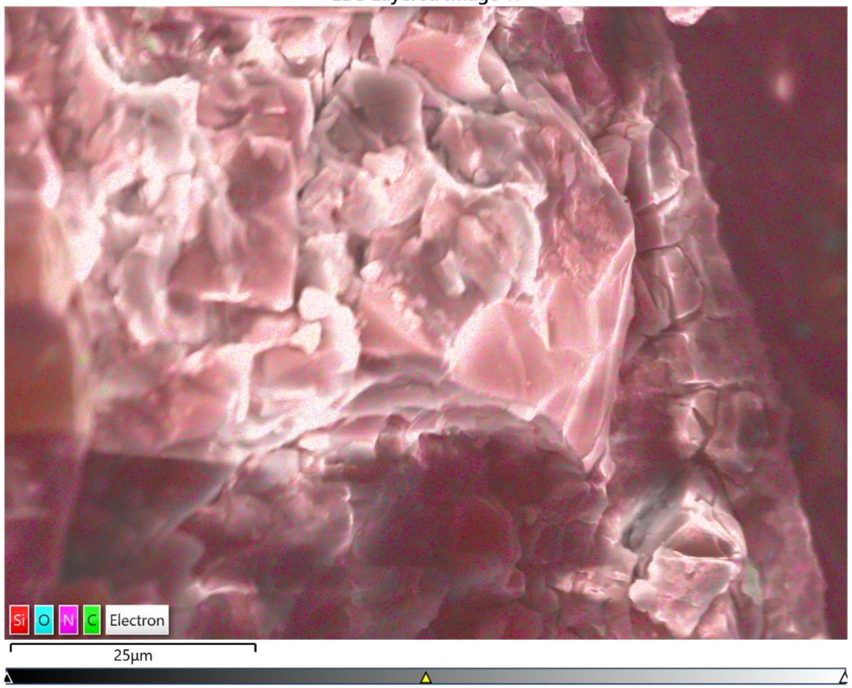
(a) (b) (c)

Test setup for 800°C quasi-static tensile test; (a) thermocouples attached to sample, (b) furnace heating up to desired temperature with thermocouples plugged in to reader, (c) tensile test being performed

S200H SiC/SiNC Creep-Fatigue Oxidation EDS Images (800°C)



EDS Layered Image 11



- **Weight percentages of undamaged SiNC matrix:**

	Wt%
Si	43.7
C	27.7
B	19.4
N	6.7
O	2.5

- **Weight percentages of portion of sample shown to the left:**

	Wt%
Si	37.0
O	33.0
C	15.6
N	14.4

Reformulated Matrix Damage Model

Modeling of brittle damage mechanism in SiC/SiC CMC constituents (the matrix and fibers)

- **The matrix modulus degradation can be described as:**

$$E_m^* = (1 - (D^p + D^c))E_m$$

- **Damage variables can be expressed as:**

$$\dot{L}_c = \frac{C_R}{\alpha}\left(\frac{K_I - K_{IC}}{K_I - \frac{K_{IC}}{2}}\right)^{\gamma} \quad \text{if } K_I \geq K_{IC}$$

Crack kinetics

$$\dot{D}^c = \frac{\pi^2}{10}(1+\nu)(5-4\nu)\frac{N}{V}L^2\dot{L},$$

Microcracking damage variable

$$\dot{D}^p = a(1 - D^p)\gamma\varepsilon^V,$$

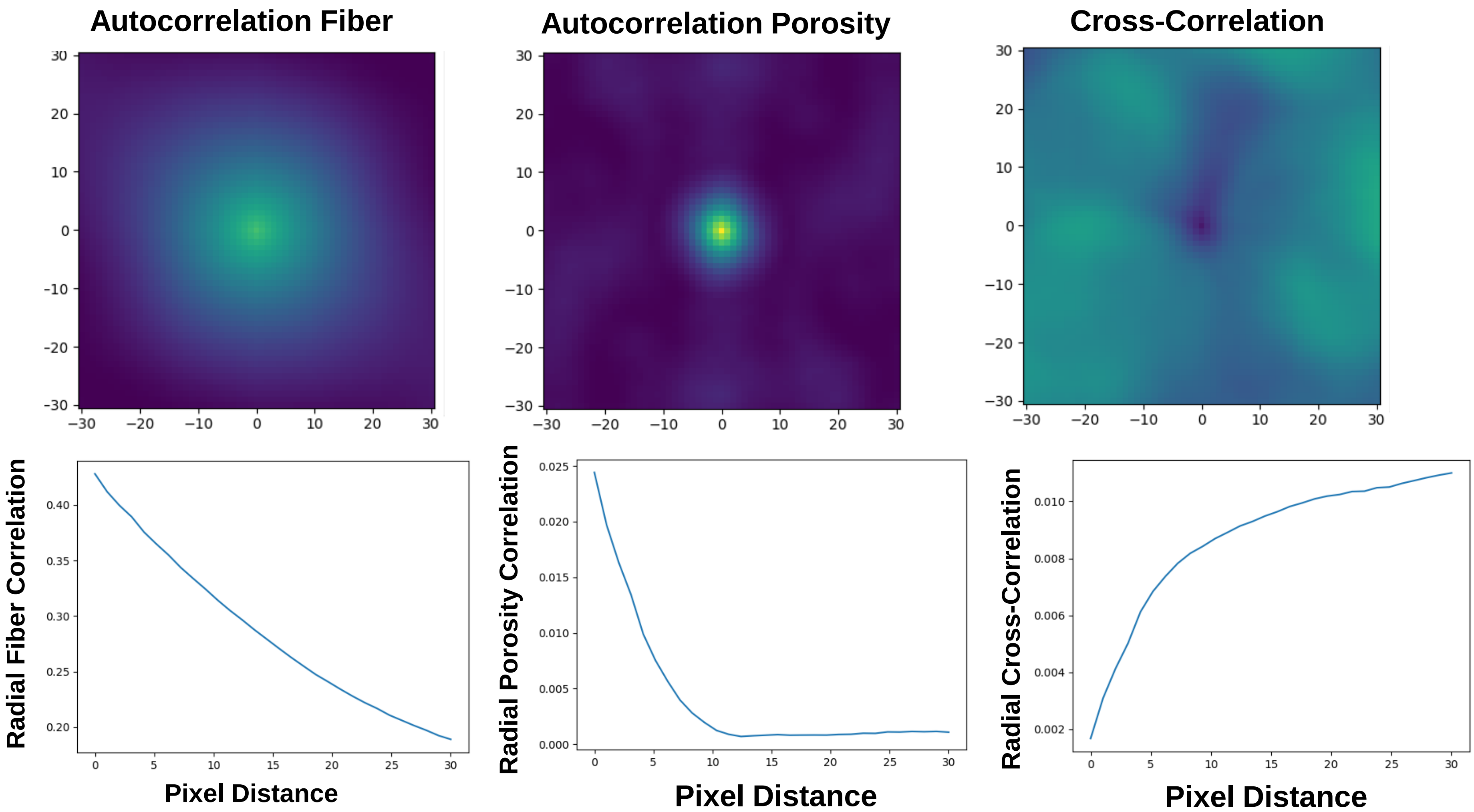
Porosity growth damage variable

$$\gamma = \frac{1}{2}\left(1 - D_p\right)\Gamma_P\, F_{dil}^{-1}\, G\left(\boldsymbol{F}_{dist}\,.\boldsymbol{I} - \frac{9}{\boldsymbol{F}_{dist}^{-1}\,.\boldsymbol{I}}\right)$$

$$\Gamma_P = \Gamma_{Po}\frac{3G}{\sigma_{eqv}}\left(\frac{\langle\sigma_{eqv} - \sigma_Y\rangle}{\sigma_{Yo}}\right)^2$$

- **Computational parametric study to investigate the influence of voids and fiber VF on the damage mechanism**

Microstructure Statistics Using Point-Correlation

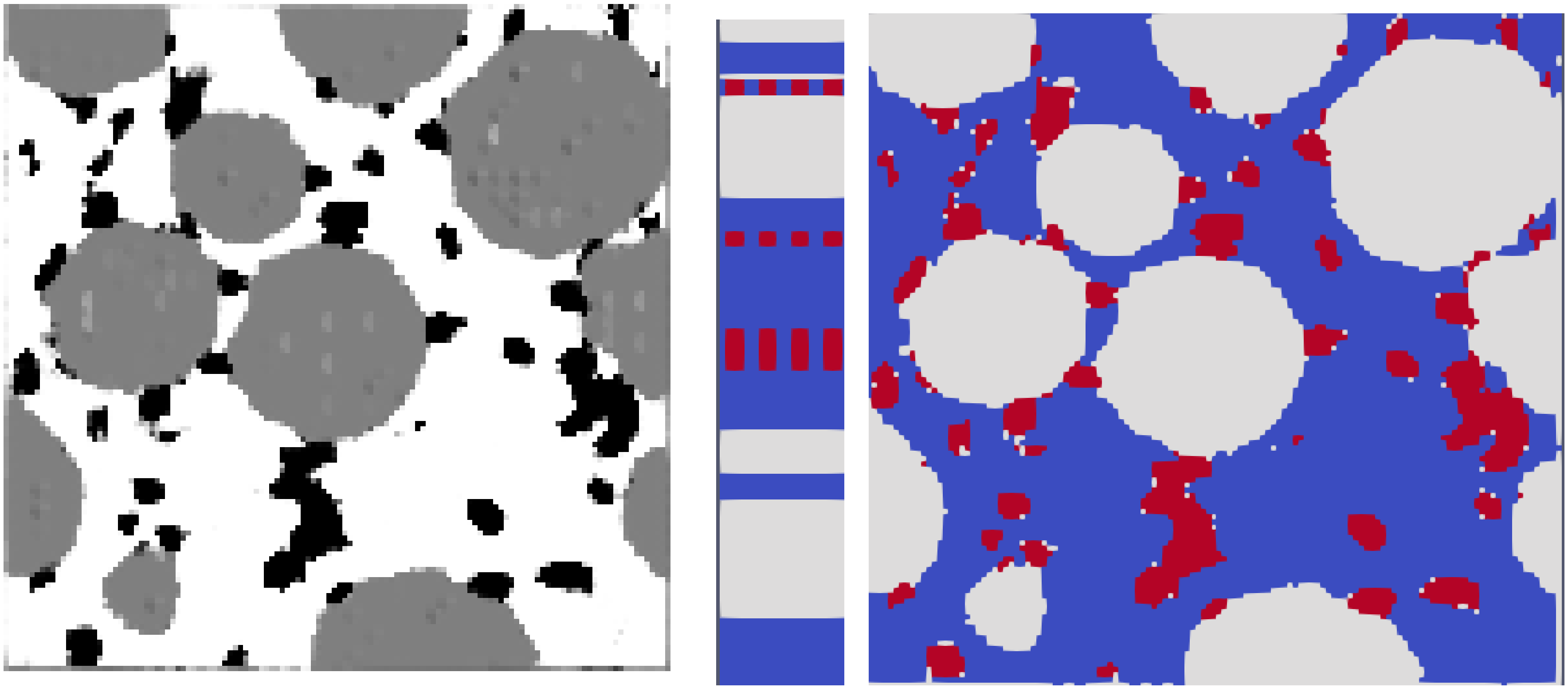


- **Computed the probability density associated with finding specific local states at two ordered material points for a given microstructure**
- **Statistical and physical descriptors preprocessing for microstructure inspired RVEs generation**

Mesh Generation for High-fidelity Generalized Methods of Cells (HFGMC)

Results: Pixel-Based Information for composite ML-based images.

X-Z Plane Y-Z Plane



• Porosity • Matrix • Fiber

- **Re-constructed DL-based images for C/SiNC and SiC/SiNC CMCs**
- **Artifacts of ML-based images in terms of fiber distribution and shape will be avoided through further optimization and tuning of the deep neural network**