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

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Overview

- Project Summary
- Motivation
- Research Objectives & Tasks
- Research Progress
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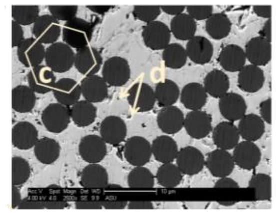
  - Multiphysics Constitutive Modeling
  - Thermomechanical Testing
  - Integrated Multiscale Framework
  - Machine Learning (ML)-based Surrogate Model
- Concluding Remarks & Future Work
- Publications
- Acknowledgements

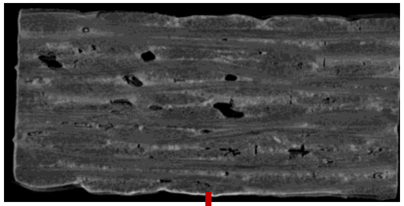
Research Objectives

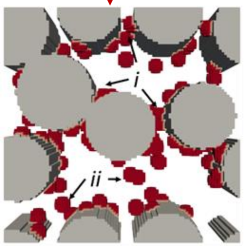
Develop a synergistic multiscale framework, integrating multiphysics constitutive models with scale specific experiments,* to understand temporospatial & scale dependent deformation, damage, & degradation mechanisms in *CMCs operating in turbine environment

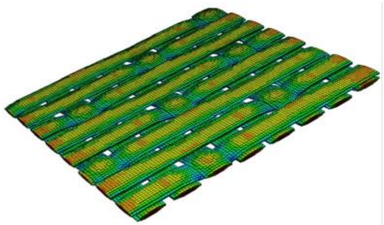
- **Accurate scale-dependent material characterization & uncertainty quantification**
- **Constitutive modeling of time-dependent damage, inelasticity, and effects of environmental degradation**
- **Efficient synergistic multiscale analysis**
- **Incorporation of developed models into commercial finite element (FE) software for CMC component analysis**
- **Reduced order model (ROM) for computationall efficiency**
- **Closed-loop testing for model calibration & validation**

Real micrographs





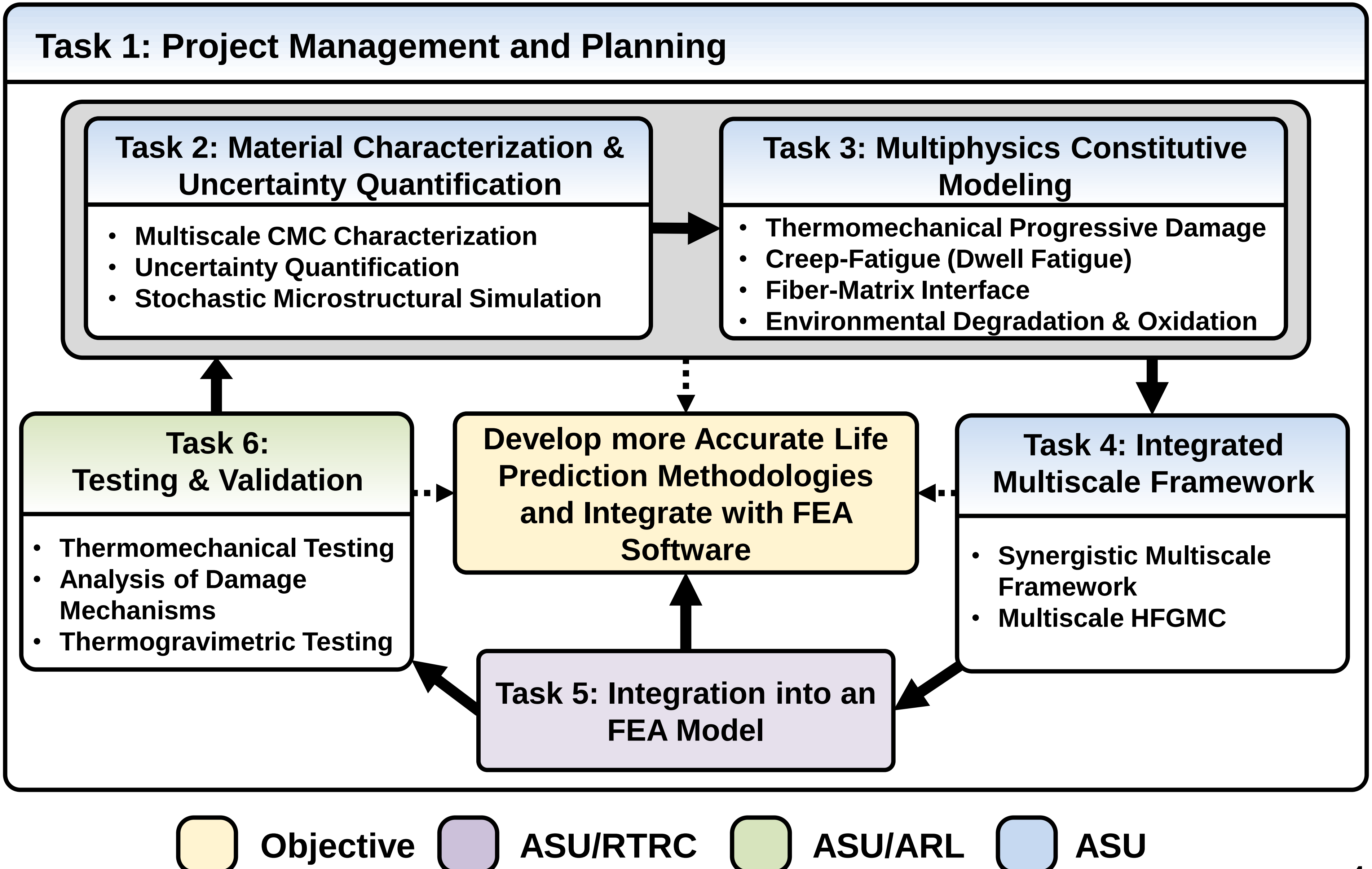




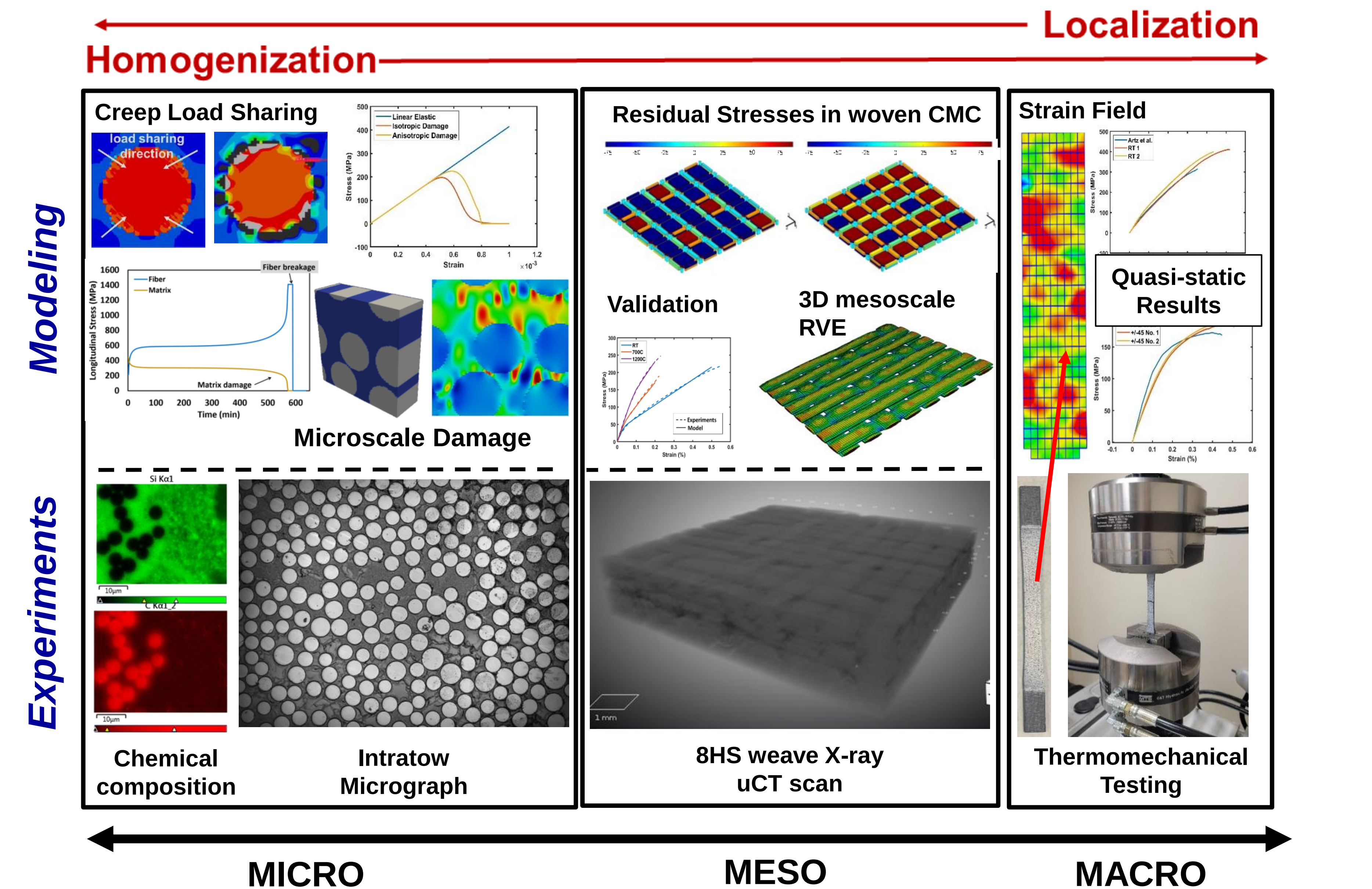
Artificial micrographs

Tensile testing

Tasks & Technical Framework



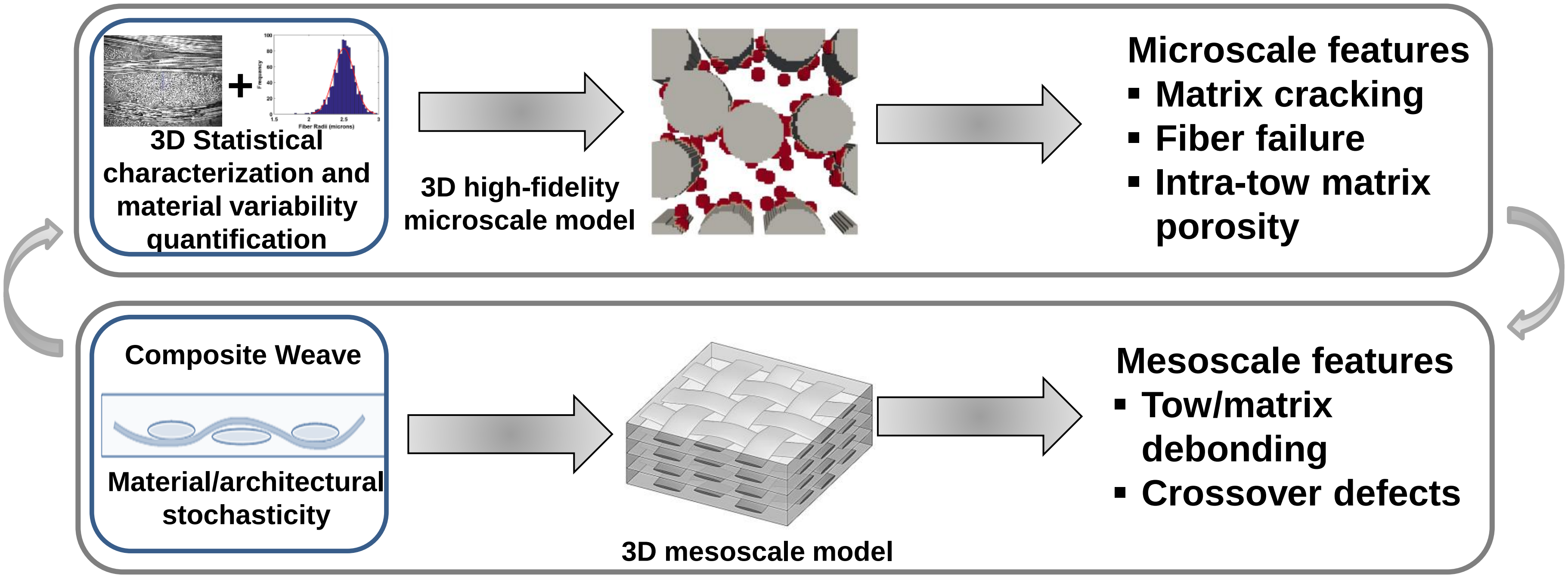
Multiphysics Multiscale Modeling Framework



Material Characterization and Uncertainty Quantification

Objective: Systematic quantification of scale-dependent architectural variability & as-produced defects to i) facilitate SRVE development & ii) investigate effects of variability on effective properties & response

- Material characterization
- Uncertainty assessment
- Generation of statistical representative volume elements (SRVEs)



Multiscale Material Characterization

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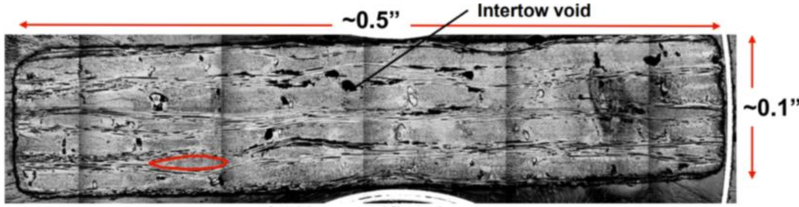
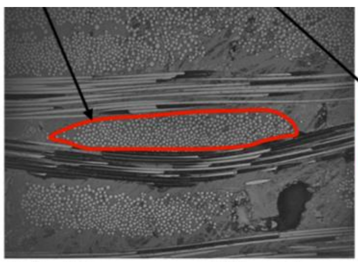
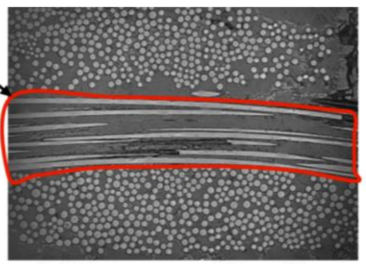


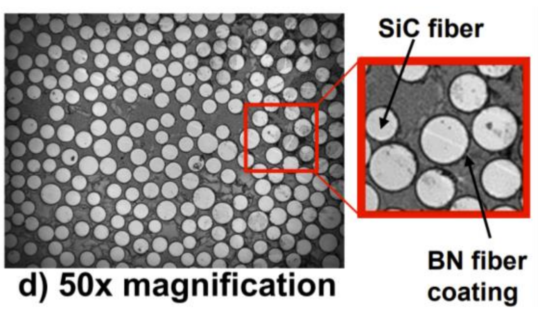
a) 5X magnification



b) 10x magnification

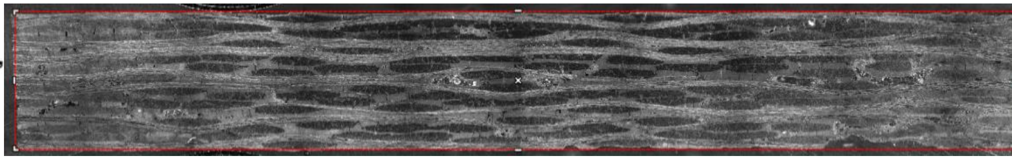


c) 20x magnification

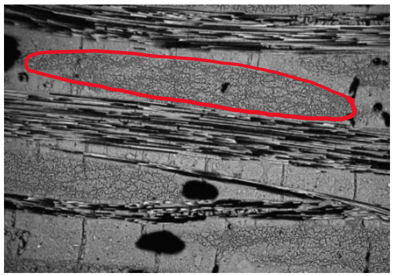


d) 50x magnification

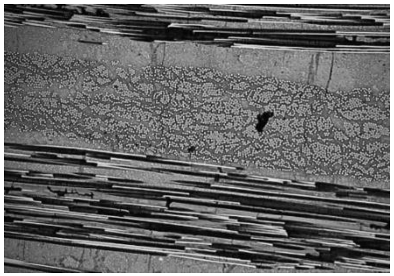
Carbon/silicon nitrocarbide



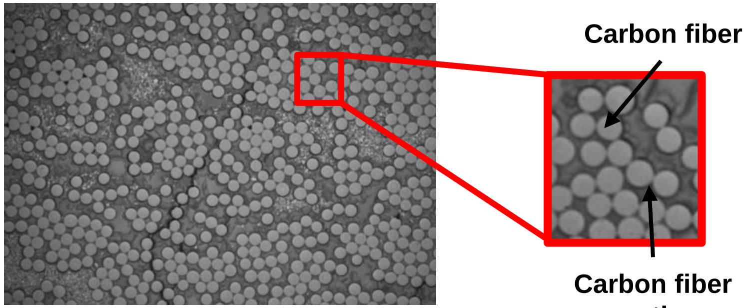
a) 5X magnification



b) 10X magnification



c) 20X magnification



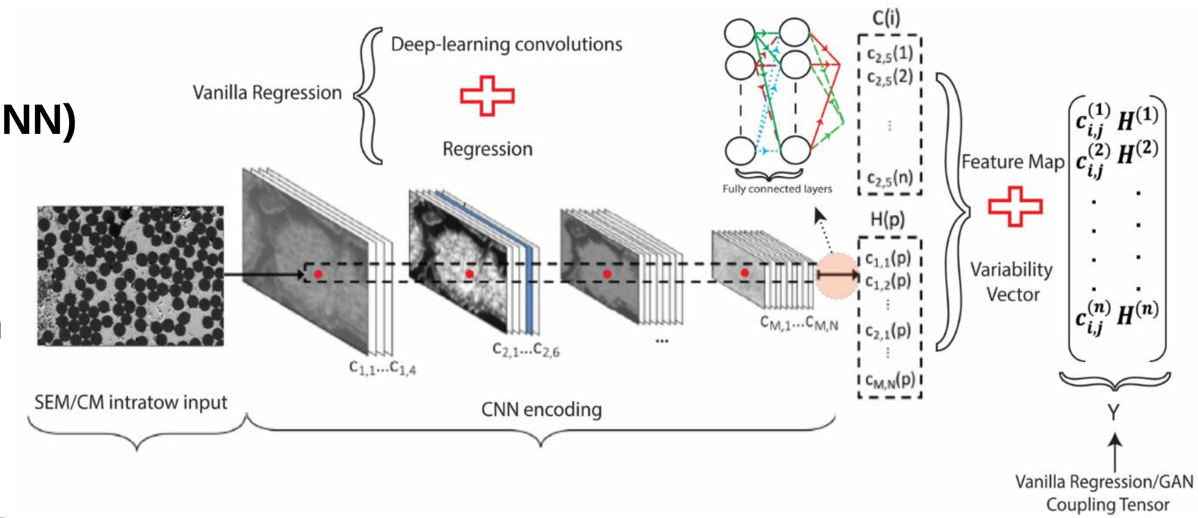
d) 50X magnification

Multiscale graphs allow quantification of architectural & defects variability at respective constituent and weave scales

Multi Deep NN–based Framework for Multiscale Microstructural Analysis

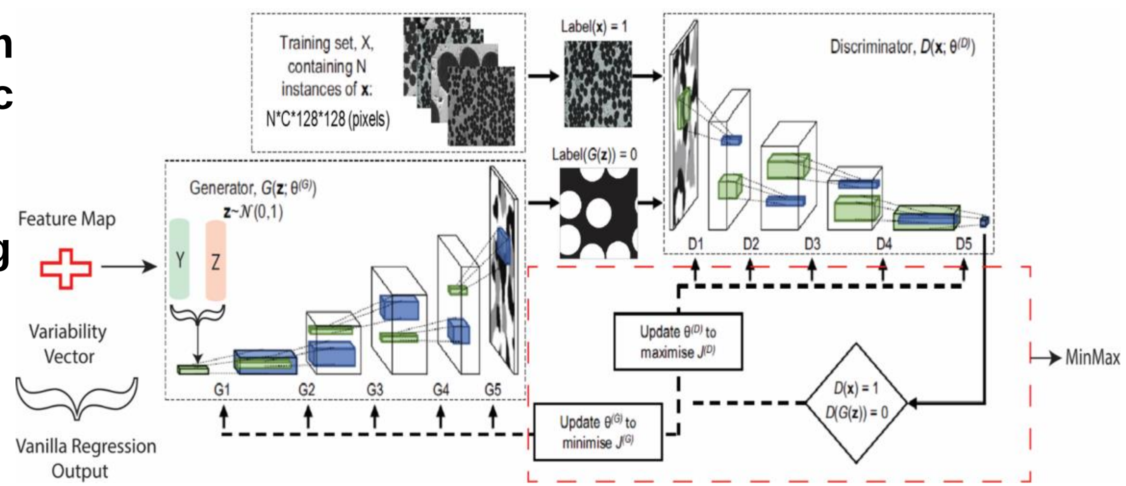
Feature extraction & variability quantification of microstructures

- **Semantic segmentation of microstructural features through Convolutional Neural Network (CNN) layers**
- **Microstructure variability quantification computed through regression layer**



Generation of High-fidelity SRVEs

- **Generator produces SRVEs from actual micrograph characteristic features & distribution**
- **Discriminator enables distinguishing between actual micrograph and generated SRVE for generator optimization**

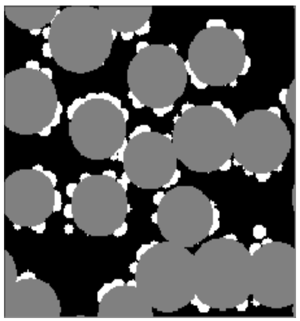


Figures are reconstructed from: 1- Holm, Elizabeth A., et al. Metallurgical and Materials Transactions A (2020)
2- Cooper, S. J. et al. npj Computational Materials (2020)

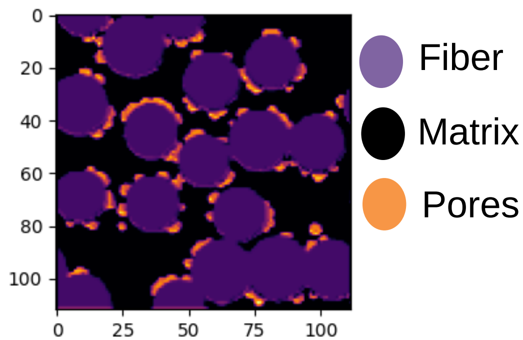
Vanilla Regression Training

Utilized previously-developed SRVE generation algorithm to train DL-based algorithm and further improve variability quantification accuracy

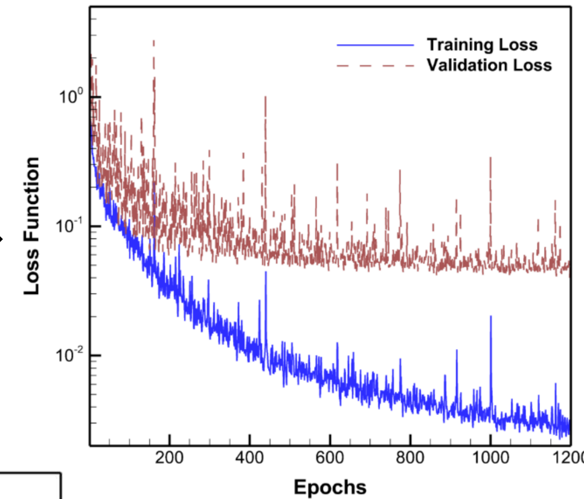
Computer-vision training microstructure

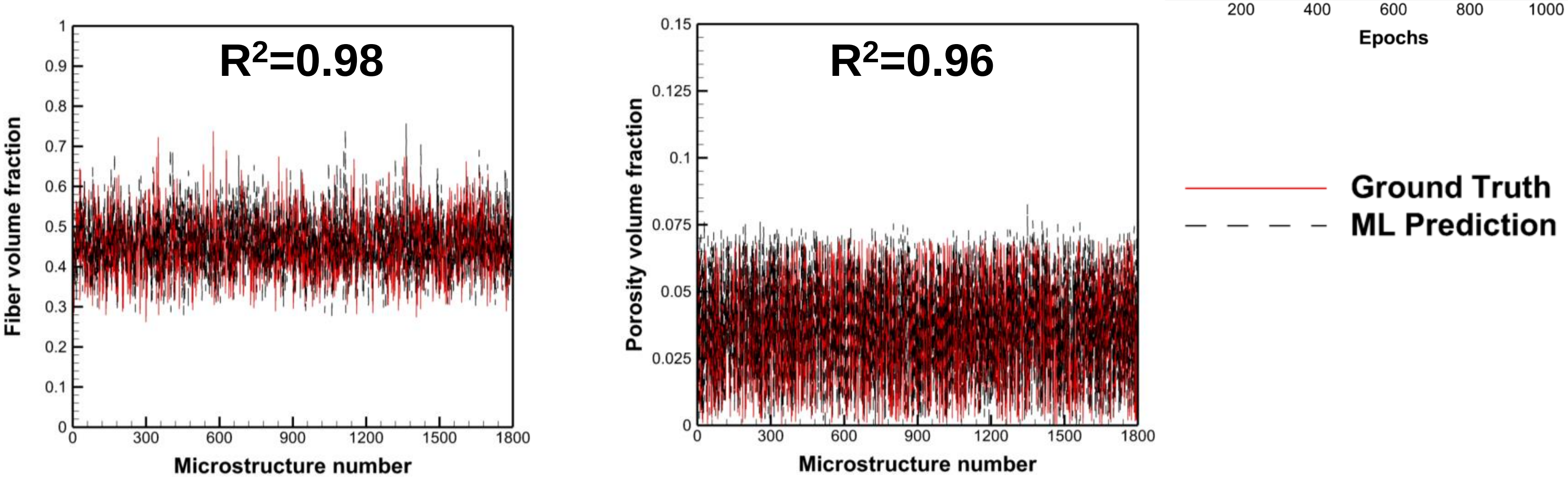


Deep-learning segmented microstructure



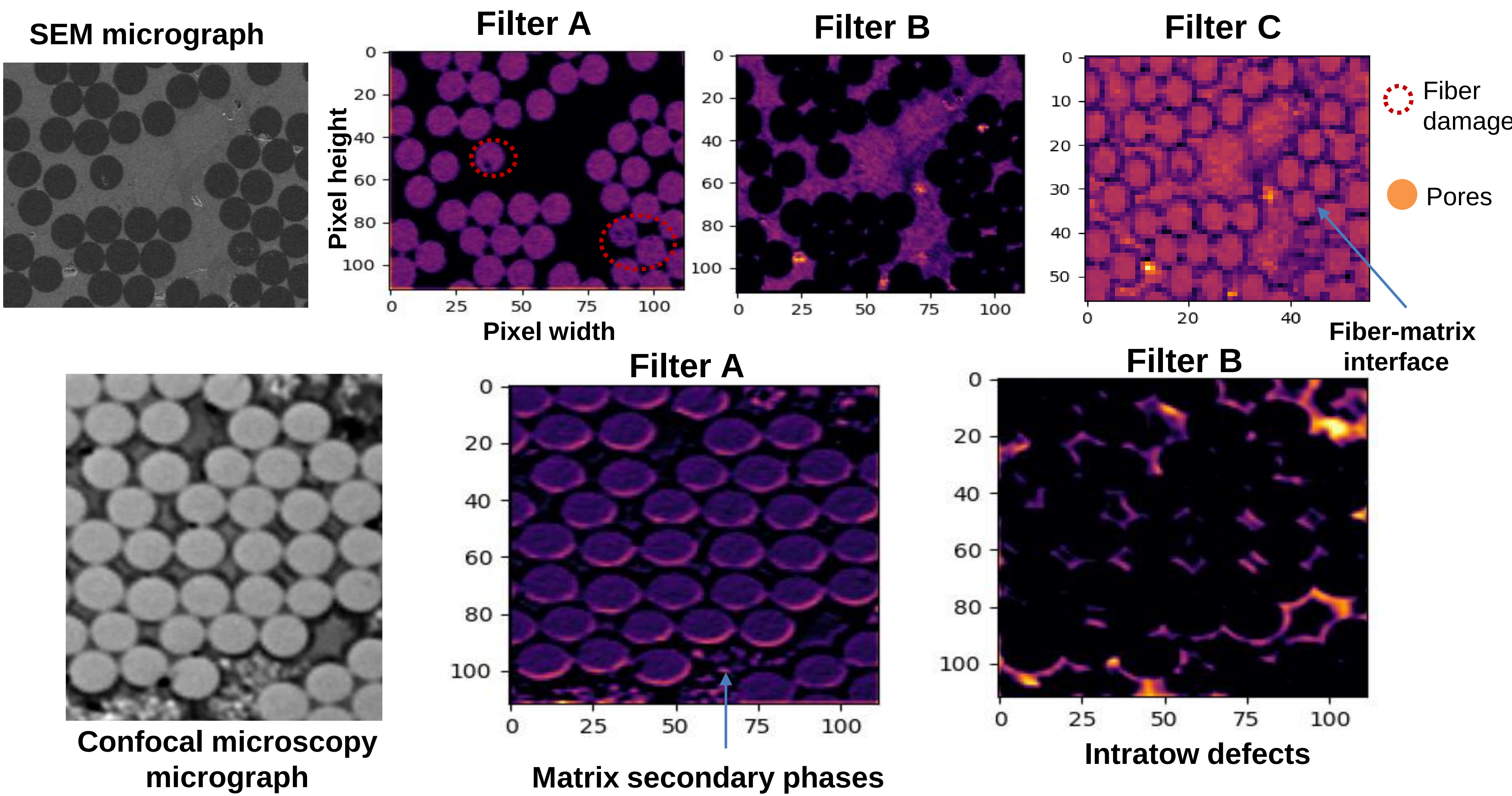
Loss function minimization





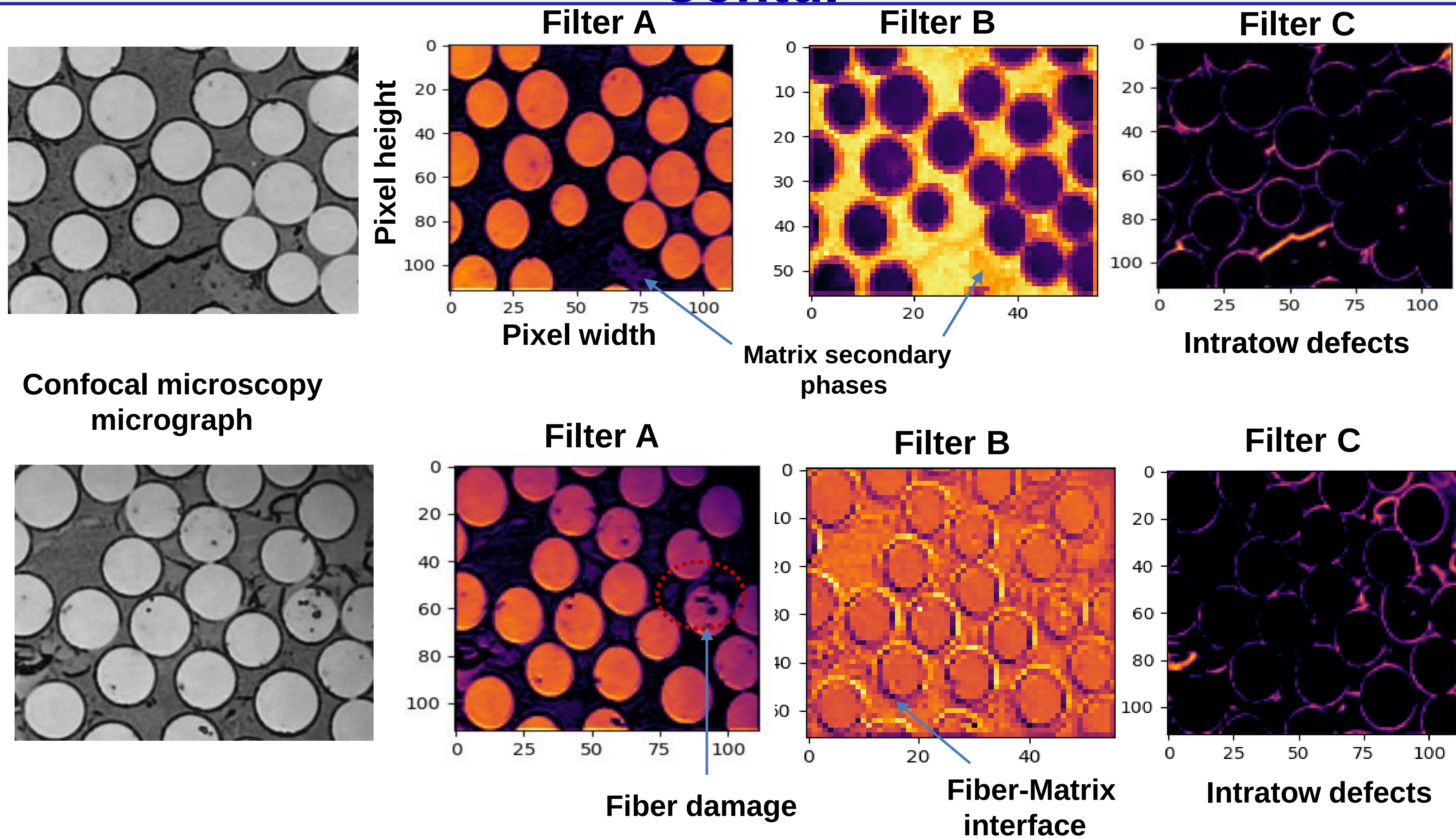
Prediction from optimized vanilla regression show high coefficient of determination (R^2) with respect to ground truth

Vanilla Regression C/SiNC Feature Maps



- Achieved semantic segmentation for matrix, fiber, fiber/matrix interface and porosity to inform high fidelity micromechanics simulations
- Captured matrix secondary phases and fiber damage regions; critical for accurate damage assessment

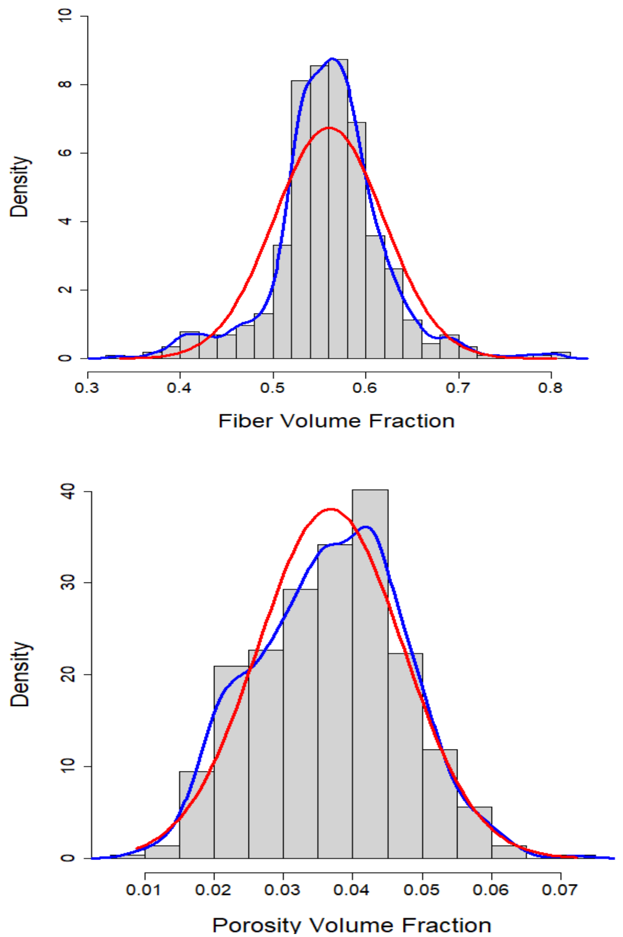
Vanilla Regression SiC/SiNC Features Map, Contd.



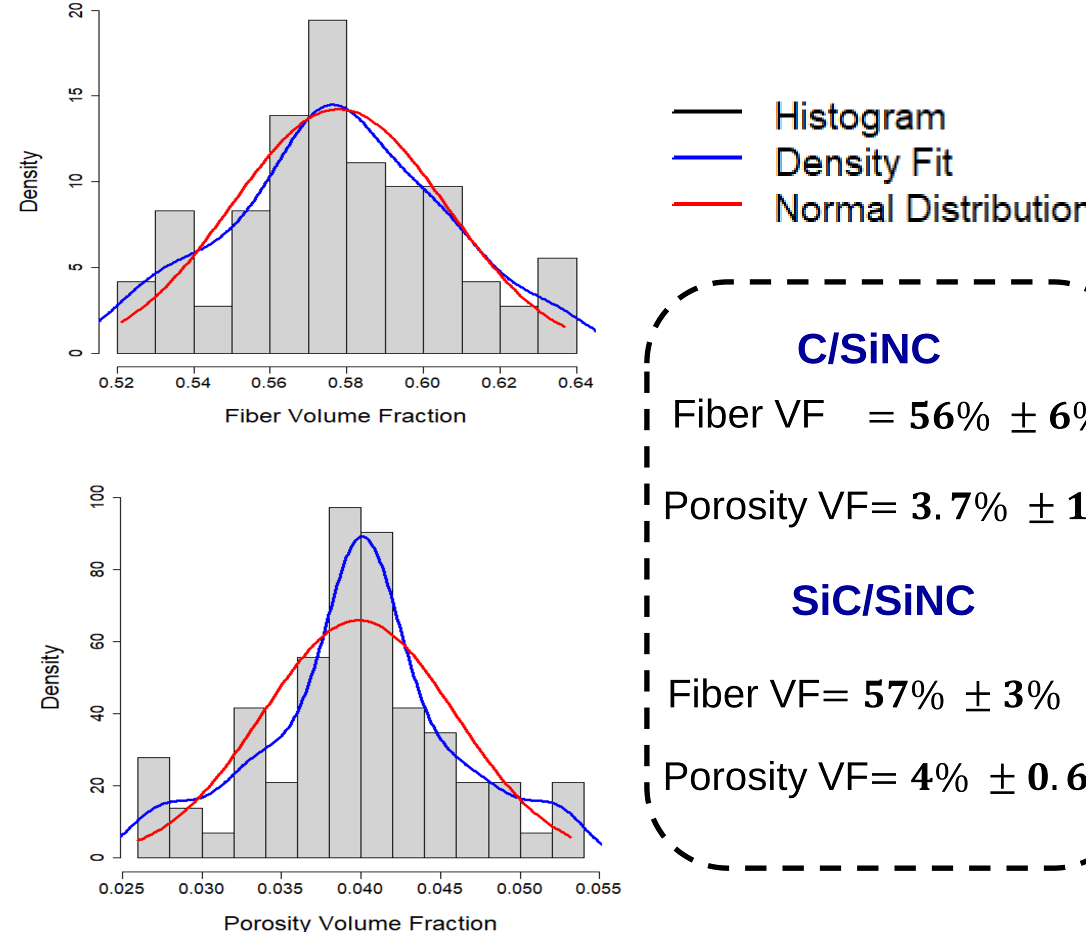
Modular deep-learning NN: Successfully segmented different microstructure variability: fiber radii, matrix crack shape & distribution and fiber-matrix chemical composition

Microstructure Variability Quantification

C/SiNC



SiC/SiNC



C/SiNC

Fiber VF $= \mathbf{56\%} \pm \mathbf{6\%}$

Porosity VF$=$ $\mathbf{3.7\%} \pm \mathbf{1\%}$

SiC/SiNC

Fiber VF$=$ $\mathbf{57\%} \pm \mathbf{3\%}$

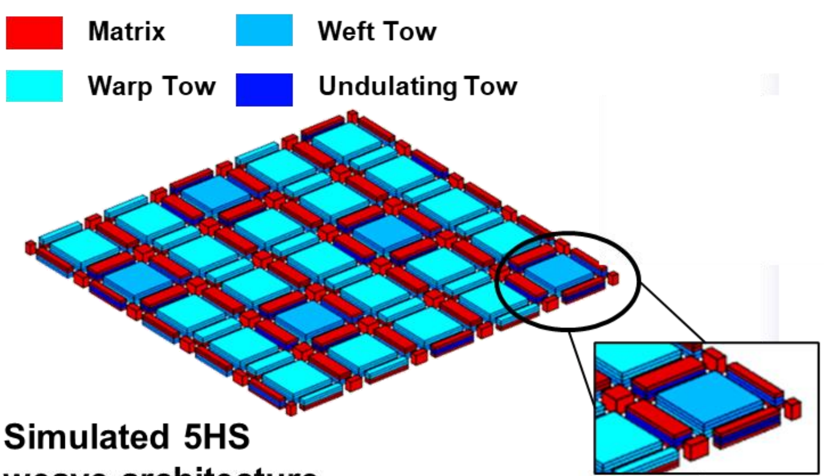
Porosity VF$=$ $\mathbf{4\%} \pm \mathbf{0.6\%}$

- **Captured microstructure variability in fiber and porosity volume fractions**
- **In-progress: fiber radius, intratow spacing, porosity shape and size, & intertow features**

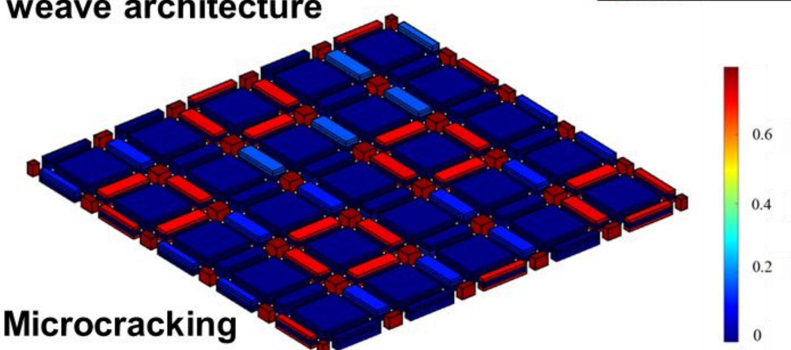
Multiscale Simulation of 5HS Woven C/SiC CMC

Thermomechanical progressive damage model accounting for crack nucleation & growth

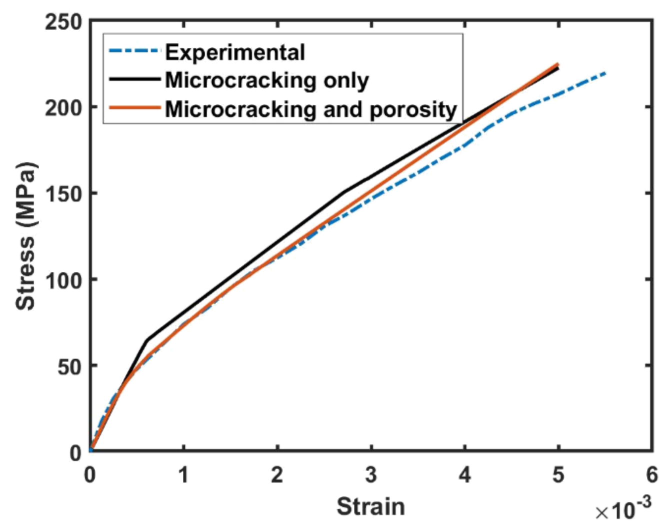
- ***Includes flaw statistics, temperature dependent material properties***
- ***Crack growth kinetics governed by fracture mechanics***



Simulated 5HS weave architecture



Microcracking damage



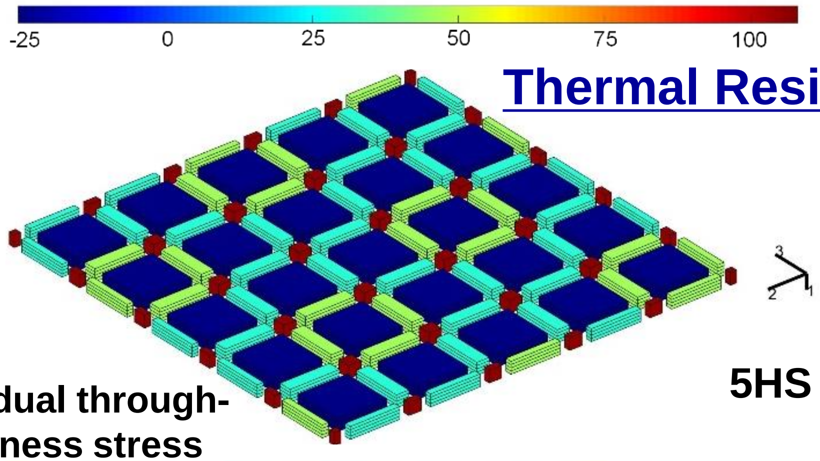
Correlation with experiments from literature (Yang et al. 2017)

Need to account for material initial damage state & residual stress effects due to cooldown during manufacturing process

Skinner, T., & Chattopadhyay, A., *Composite Structures* (2021)

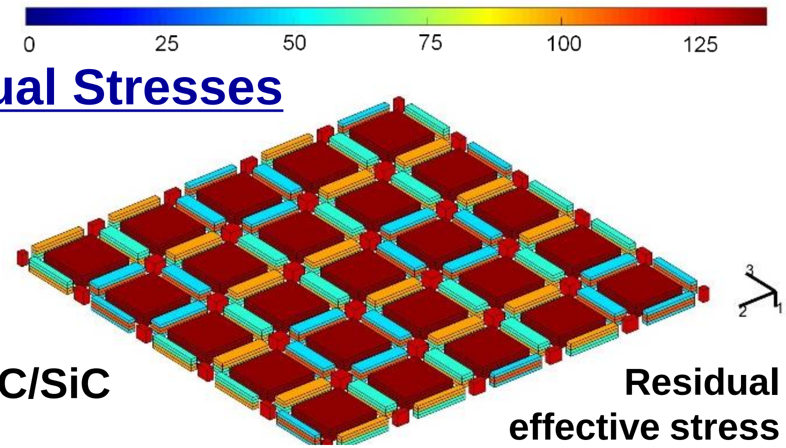
Reformulated Framework with Cooldown Effects

Thermal Residual Stresses

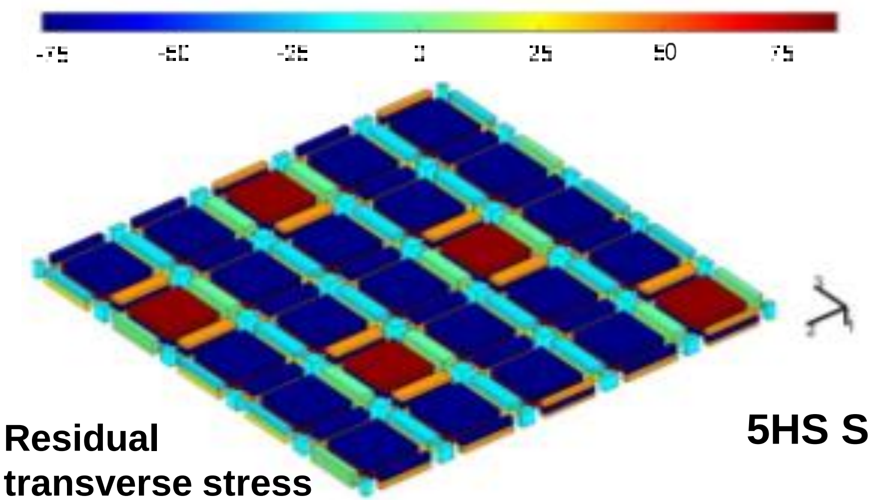


Residual through-thickness stress

5HS SiC/SiC

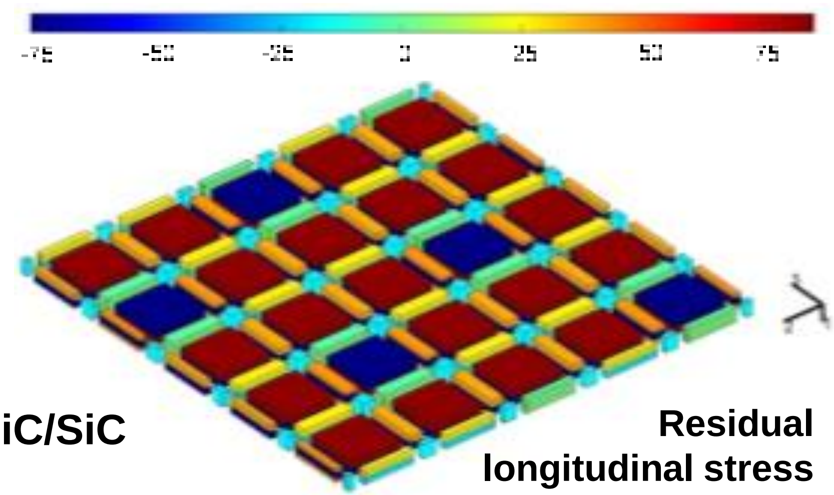


Residual effective stress



Residual transverse stress

5HS SiC/SiC



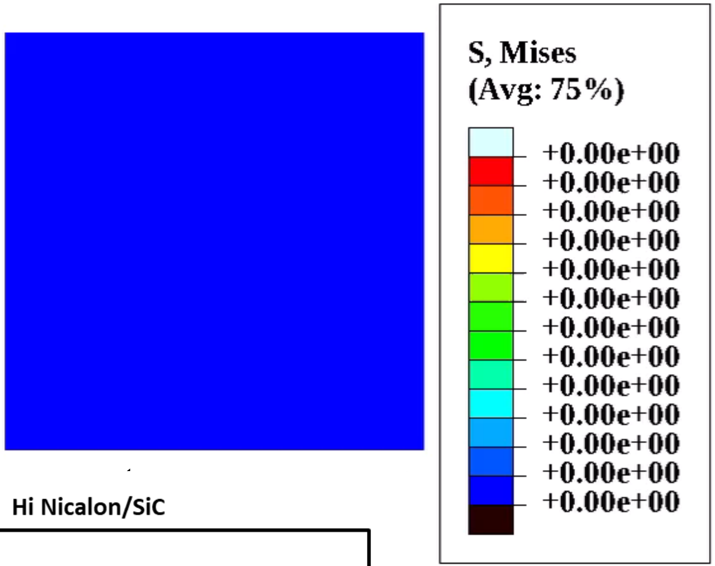
Residual longitudinal stress

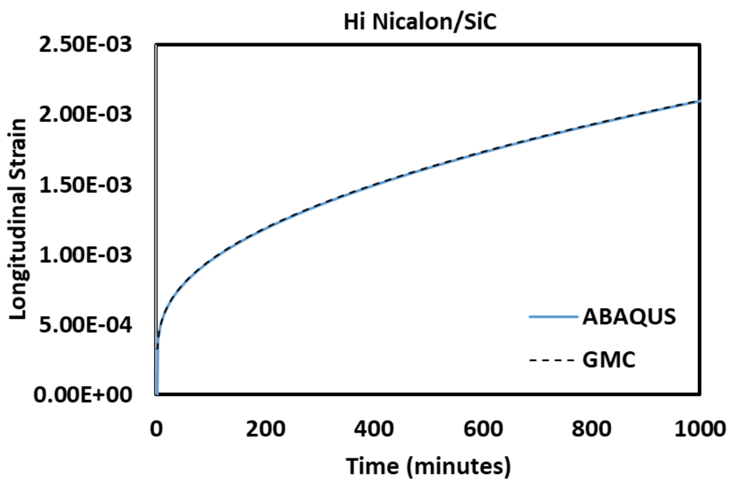
Areas with high residual tensile stress have shrinkage cracks; high stress areas in cooldown framework accumulate damage & exhibit degraded initial properties in damage direction

High-fidelity FE Creep Modeling

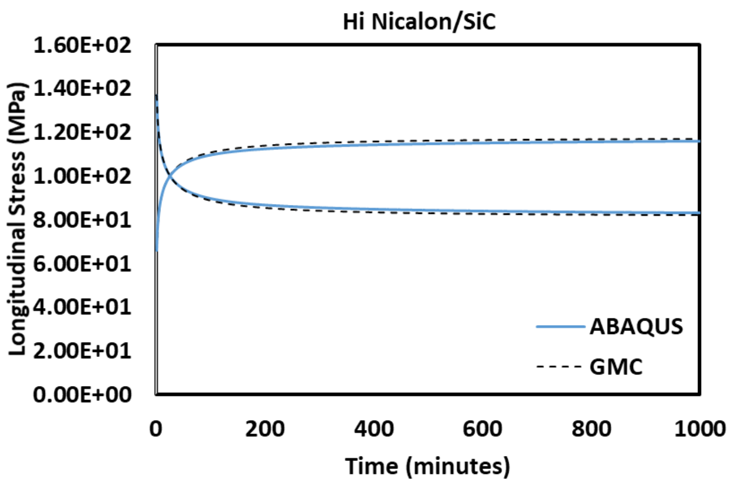
3D coupled viscoplasticity-damage model:

- Norton-Bailey creep power law
- Hill orthotropic plastic potential
- Arrhenius temperature dependence
- Associative flow rule
- Time- and strain-hardening formulations
- Fracture mechanics-informed matrix damage model
- Curtin progressive fiber damage model





Total longitudinal strain vs. time



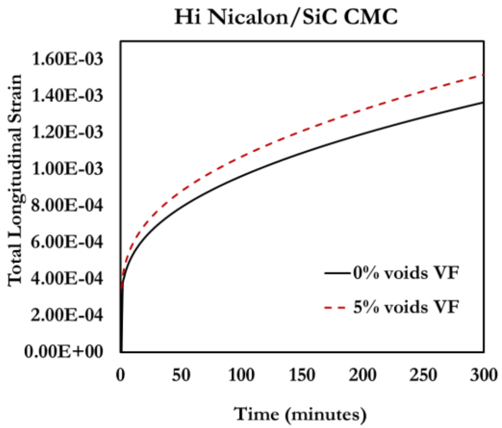
Constituent longitudinal stress vs. time

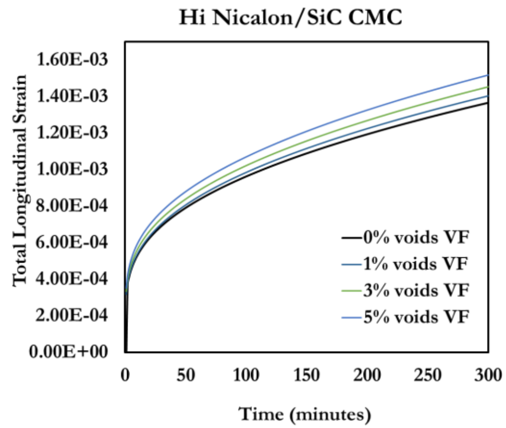
- Captured transient creep stage due to large constituent creep mismatch, followed by steady-state stage
- Excellent agreement with CMC total longitudinal strain & constituent longitudinal stress time-history

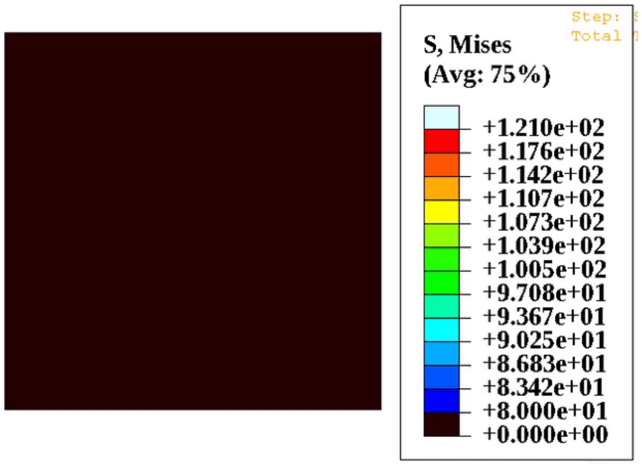
High-fidelity FE Creep Modeling, Contd.

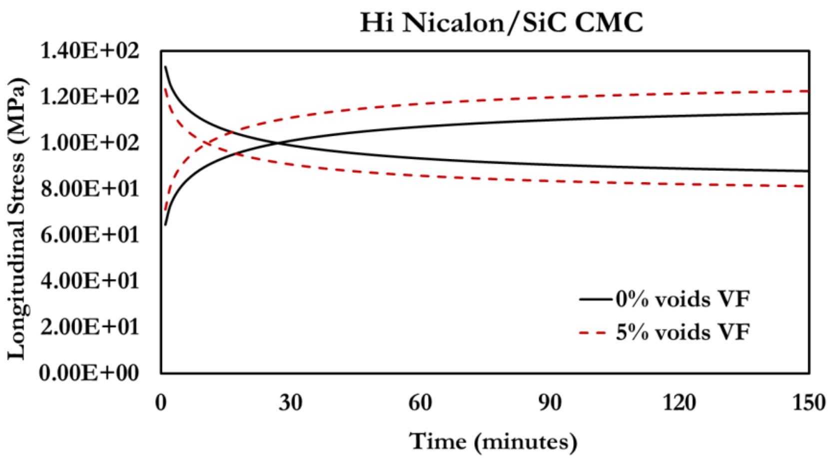
Effects of intratow porosity on creep behavior

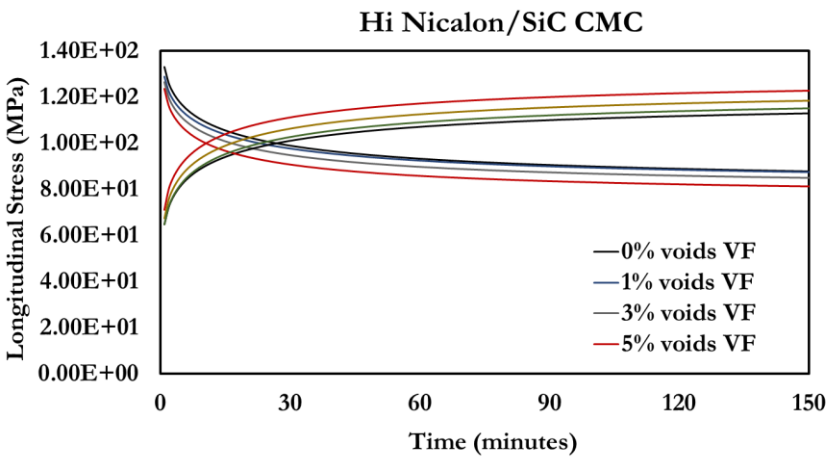
Prescribed loading: 100 MPa (constant), 1300 °C











Presence of intratow voids affects load transfer mechanism between constituents & results in complex stress "hot spots" in vicinity of voids - *potential damage initiation sites*

Damage-diffusion Oxidation Coupling

Matrix cracks create passages for oxygen to diffuse into material

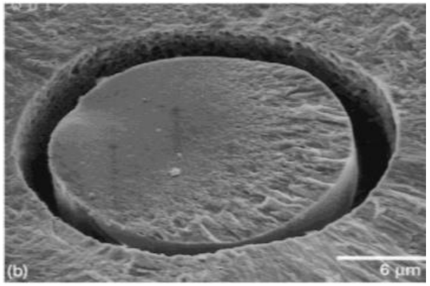
- Oxidation of fiber interphase or fusion of SiC fiber to SiNC matrix impairs load transfer
- Oxidation reaction of oxygen-exposed SiNC matrix activates at extreme temperatures, resulting in a multi-regime response

Physics-based modeling

- Model oxidation coupling through the chemical reaction source terms for concentrations of oxygen and material
- Model damage-driven diffusion through approximations of the partial differential equations

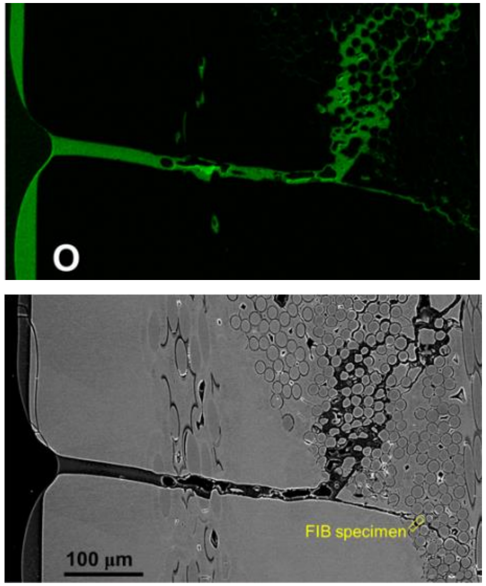
Model under development to address complex coupling between anisotropic damage, diffusion, crack closure, & oxidation of the fiber-matrix interphase at the microscale

Oxidation of fiber interface



Jacobson (1999) "High-Temperature Oxidation of Boron Nitride: II, Boron Nitride Layers in Composites".

Oxygen diffusing through cracks



Terrani (2014) "Silicon carbide oxidation in steam up to 2 MPa". Journal of the American Ceramic Society.

Damage-diffusion Oxidation Coupling, Contd.

Five degrees of freedom (DOFs) per node: displacement (x, y, z), concentration (O_2, BN)

Governing equations:

For $c_{(O_2)}$ DOF: $\dot{c}_{(O_2)} - \vec{\nabla} \cdot \left(\boldsymbol{D} \vec{\nabla} c_{(O_2)} \right) + R c_{(BN)} c_{(O_2)} = 0$
For $c_{(BN)}$ DOF: $\dot{c}_{(BN)} + R c_{(BN)} c_{(O_2)} = 0$
For displacement DOFs: $\nabla \cdot \sigma = 0$

Oxidation reaction 1: $2BN(s) + \frac{3}{2} O_2(g) \rightarrow B_2O_3(l) + N_2(g)$

Diffusion crack path matrix:

$$\boldsymbol{P} = \begin{bmatrix} \frac{d_{22}h_{22} + d_{33}h_{33}}{2} & 0 & 0 \\ 0 & \frac{d_{11}h_{11} + d_{33}h_{33}}{2} & 0 \\ 0 & 0 & \frac{d_{22}h_{22} + d_{11}h_{11}}{2} \end{bmatrix}$$

	For SiC:	***For Interphase:***
Stress:	$\sigma = \mathbf{MC}\varepsilon$	$\sigma = \left(1 - \frac{c_{(BN)}}{c_{(BN)}^{max}} \right) \mathbf{C}\varepsilon$
Effective oxygen diffusivity:	$\boldsymbol{D} = \boldsymbol{P} \cdot D_{air_{(O_2)}}$	$\boldsymbol{D} = \left(1 - \frac{c_{(BN)}}{c_{(BN)}^{max}} \right) D_{air_{(O_2)}} \boldsymbol{I}$

In-situ Tensile Testing

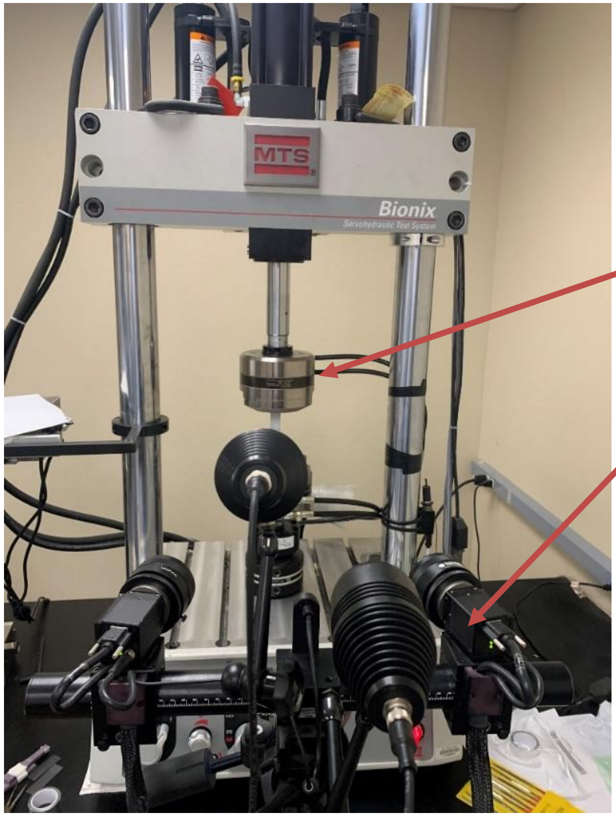
Experimental set-up

DIC speckle pattern

Amteco Furnace (>1400 ^{o}C)

- Two independent heating zones for better temperature uniformity control
- View port access for in-situ (DIC) experiments

30kN MTS load frame



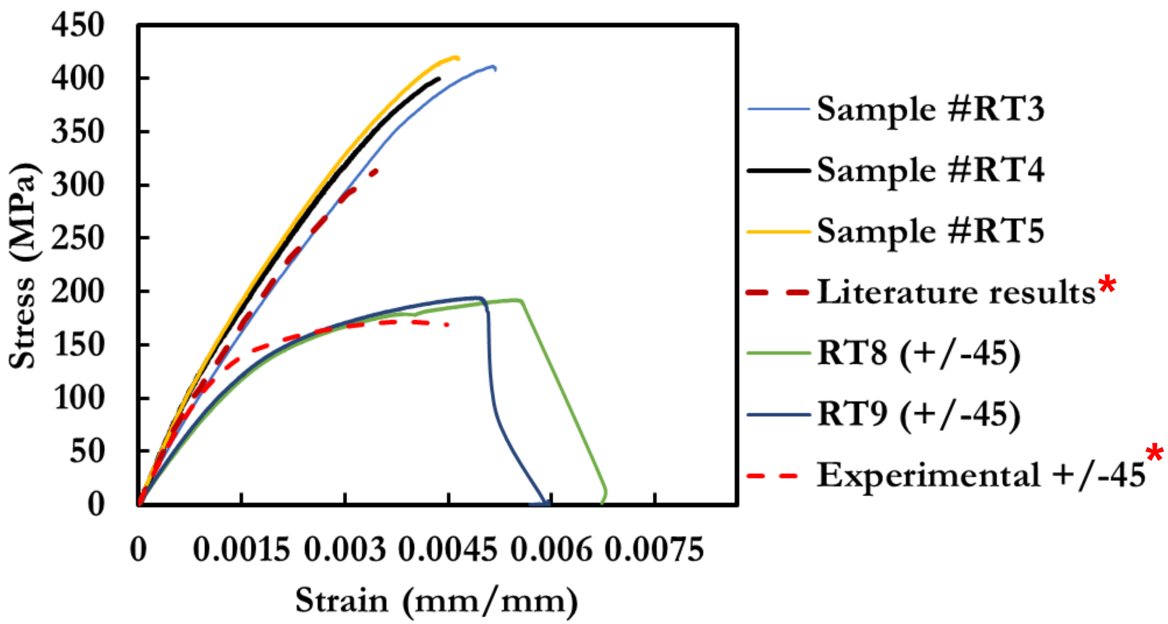
Hydraulic grip system

Digital image correlation

High & room temperature quasi-static (QS) & creep testing for SiC/SiNC using MTS load frame and *in-situ* digital image correlation (DIC) technique

Quasi-Static Tensile Testing, Contd.

SiC/SiNC CMC stress-strain response and strength



- **Loading conditions:**
QS strain rate = 1e-5/sec
- **Temperature conditions:**
Room temperature = 24 °C
- **Gauge region dimensions:**
99.0 x 10.2 x 2.5 (mm)

Average tensile strength = 409.34 MPa (0/90°) & 193.24 MPa (+/-45°)

Average failure strain = 0.4731% (0/90°) & 0.52 % (+/-45°)

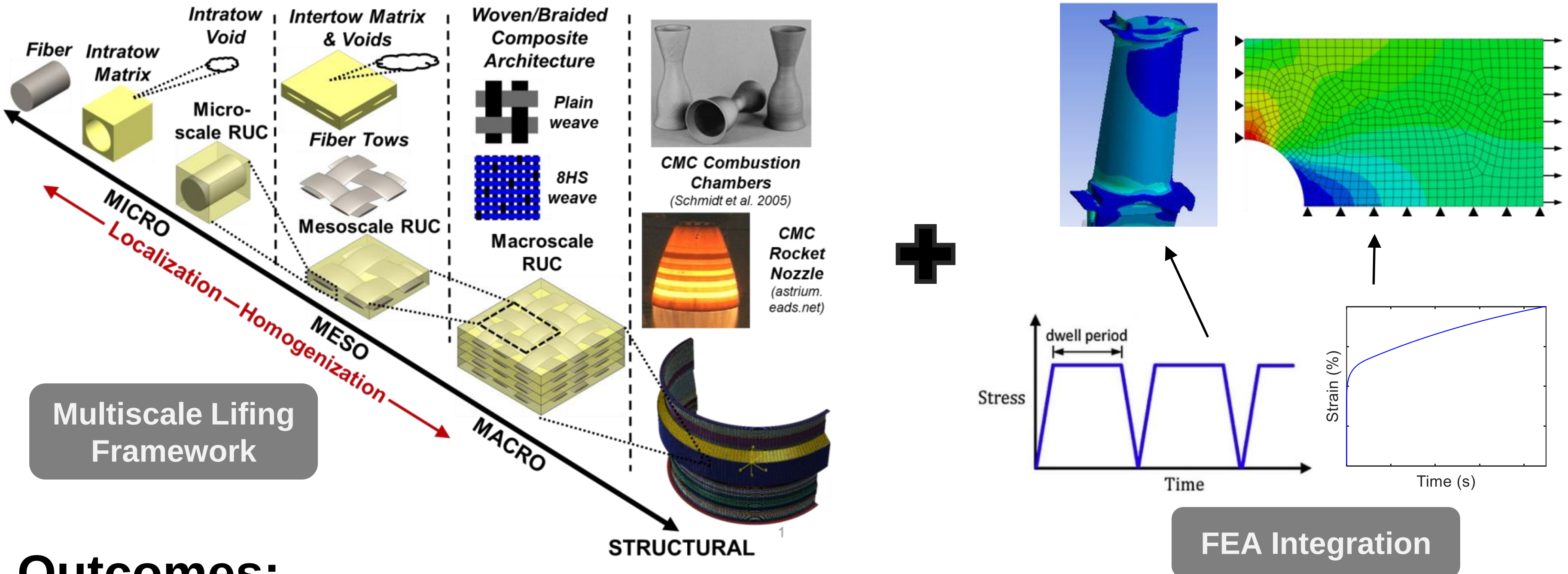
Results show good agreement with data from literature

*Artz et. al, 2020, *International Journal of Solids and Structures*, *202*, pp.195-207.

Integrated Multiscale Framework

Challenge & Goal:

Raytheon's role includes evaluating multiscale models for industrial applications (i.e., relevant materials, geometries, loads)



Outcomes:

- **Assessment of accuracy and efficiency of lifing model for material systems, geometries, and loads relevant to RTX**
- **Technology readiness level (TRL) evaluation of modeling framework**
- **Validate simulation results against in-house lifing tools**

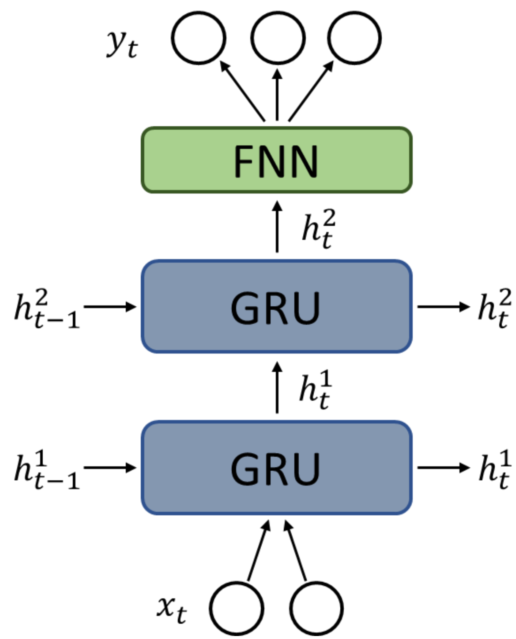
Machine Learning Surrogate Model

Approach:

Surrogate models will help bridge gap between high-fidelity multiscale models and industrial application

- **Efficiently approximate output of physics-based models**
- **Neural-network based surrogate model – trained on experimental and simulation data**
- **Physics-based regularization to enforce physical laws**

Neural network-based surrogate model architecture

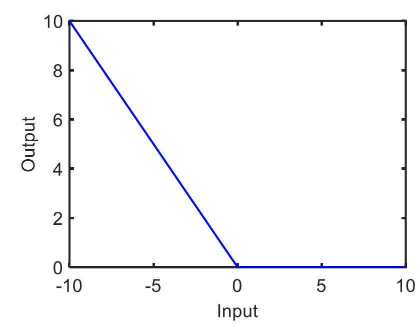


Physics-based regularization

$$l_T = \lambda_{MSE} l_{MSE} + \lambda_P l_P$$

$$l_{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - y_i^p\right)^2$$

$$l_P = \overline{ReLU\left(-\dot{w}^p\right)}$$



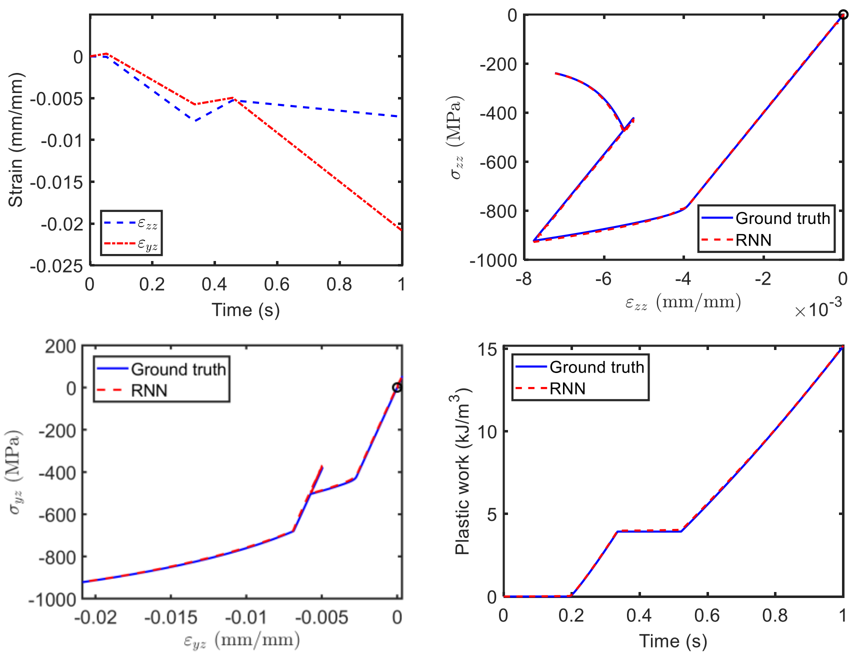
Surrogate model will run much faster than numerical solution - making large-scale multiscale simulations more feasible

Machine Learning Surrogate Model, Contd.

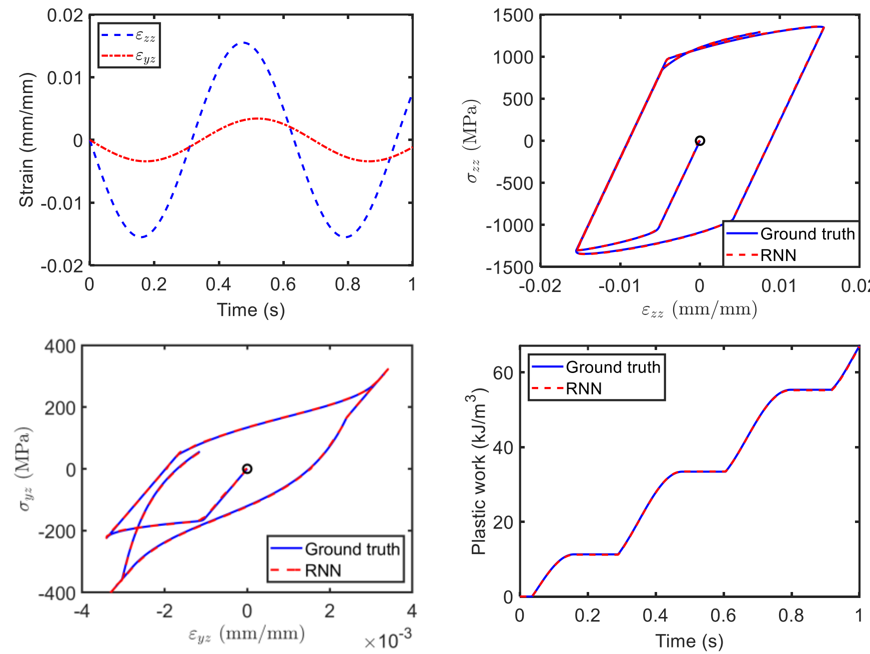
<u>Results</u>:

As proof-of-concept, surrogate model trained and evaluated using nonlinear plasticity numerical model

Validation results – Piecewise linear reverse loading



Validation results – Cyclic random amplitude, random frequency loading



Excellent agreement between ML surrogate and training data

**Borkowski, Sorini and Chattopadhyay (2021)*

Surrogate Model for Woven CMC Material System

Surrogate model developed, trained, and tested for woven CMC under cyclic loading conditions

- **RNN-based surrogate model prediction includes homogenized constitutive response of multiple constituents (fiber, matrix, interphase)**
- **Physics-based regularization to enforce physical laws (e.g., tangent stiffness matrix positive semi-definiteness) and maintain linear elastic unloading**
- **Nonlinear tensile cyclic loading response of plain weave CMC governed by progressive matrix damage model**

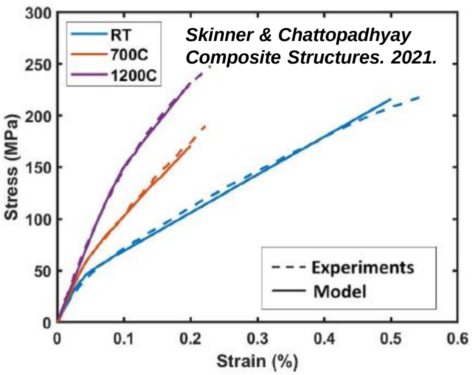
Physics-based regularization

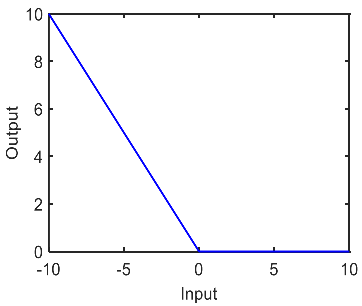
$$l_T = \lambda_{MSE} l_{MSE} + \lambda_{TM} l_{TM} + \lambda_{PSD} l_{PSD}$$

$$l_{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(\sigma_i - \sigma_i^p\right)^2 \qquad l_{TM} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial \sigma_i}{\partial \varepsilon_i} - \frac{\partial {\sigma_i}^p}{\partial \varepsilon_i}\right)^2$$

$$l_{PSD} = \overline{ReLU\left(-\frac{\partial \sigma_i^p}{\partial \epsilon_i}\right)}$$

CMC damage model





Surrogate Model for Woven CMC Material System, Contd.

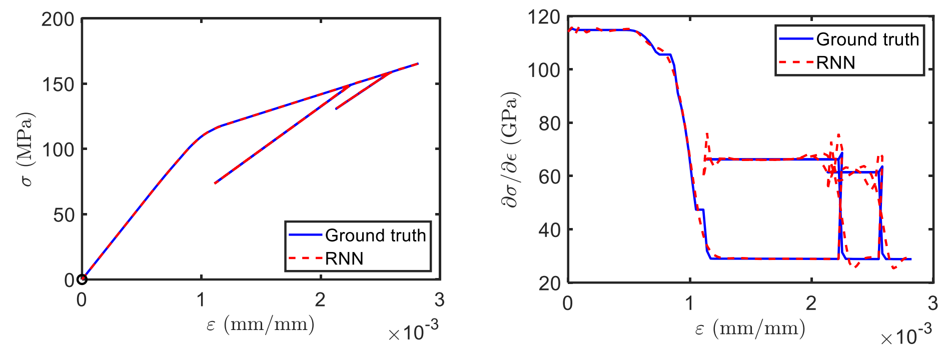
Surrogate model shown to perform well in predicting CMC cyclic behavior, including unloading

- Training data generated using Multiscale Generalized Method of Cells (MSGMC) micromechanics model

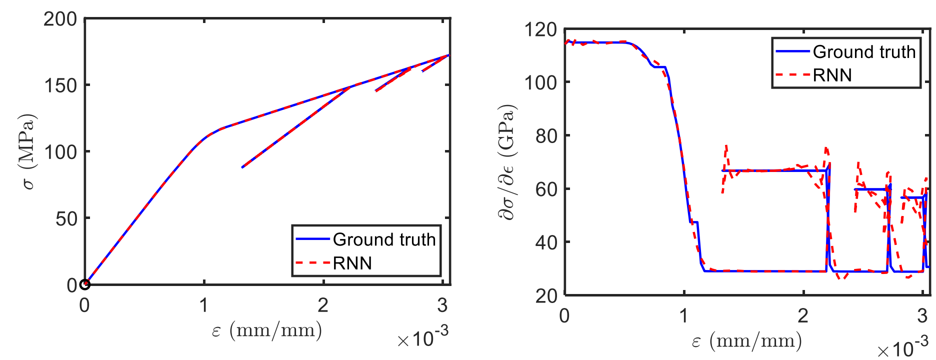
- Uniaxial load / unload cycles applied (up to four) at random points during loading and of varying unload magnitudes

Surrogate model validation

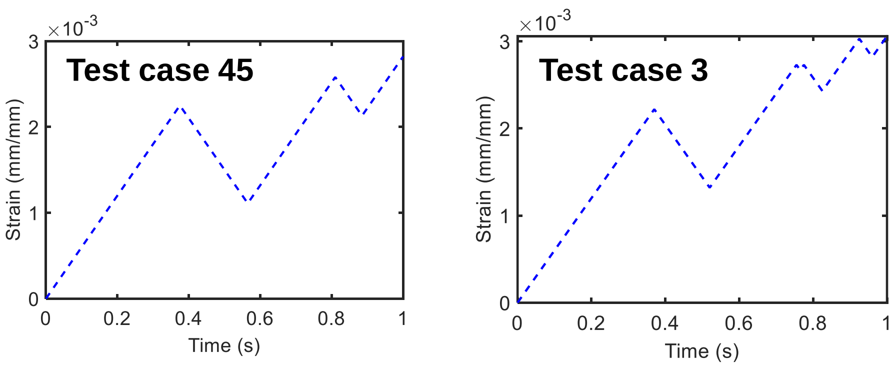
Test case 45



Test case 3



Sample loading histories



Concluding Remarks

- Developed concurrent & efficient high-fidelity multiscale simulation methodology
- Characterized scale-dependent architectural variability & defects in C/SiNC and SiC/SiNC CMCs material systems using SEM, EDS, X-ray Micro-CT, and confocal microscopy
- Developed microstructure generation algorithm accounting for material variability and defects, captured from detailed characterization study
- Developed ML-based techniques to facilitate image segmentation, scale-dependent variability quantification, and SRVE generation
- Developed multiscale cooldown framework and temperature-dependent damage model - i) simulates manufacturing-induced damage & thermal residual stresses; ii) captures nonlinear thermomechanical response
- Developed 3D orthotropic viscoplastic creep constitutive model & implementation in i) GMC micromechanics framework; ii) ABAQUS commercial FEA via UMAT
- Formulated oxidation model with complex coupling between anisotropic damage, diffusion, crack closure, & hygrothermal effects
- Developed NN-based surrogate model to facilitate computationally efficient information transfer across multiple analysis length scales
- Conducted *in-situ* quasi-static tensile testing using digital image correlation

Future Work

- **Development of conditional generative adversarial network for experimentally-inspired SRVEs**
- **Hybrid μCT-microscopy segmentation approach for mesoscale 8HS SiC/SiNC CMC SRVE**
- **High-fidelity SRVE simulations including damage and creep**
- **Integration of oxidative-damage model into multiscale framework**
- **Extension of ML-surrogate model to account for viscoplasticity and damage anisotropy**
- **Dwell-fatigue testing & modeling**

Publications

Journals

1. Borkowski, L., Sorini, C., & Chattopadhyay, A., Recurrent Neural Network-Based Multiaxial Plasticity Model with Regularization for Physics-Informed Constraints. *Computers and Structures*, 2022.
2. Khafagy, K., Datta S. & Chattopadhyay, A., “Multiscale Characterization and Representation of Variability in Ceramic Matrix Composites", *Journal of Composite Materials,* 2021.
3. Khafagy, K., Sorini, C., Skinner, T. & Chattopadhyay, A., “Modeling Creep Behavior in Ceramic Matrix Composites”, *Ceramics International,* 2021.
4. Khafagy, K., Venkatesan, K. & Chattopadhyay, A., “Microstructural damage and failure analysis of composites using finite element and high-fidelity micromechanics solvers”. Composite Structures*,* (in preparation).
5. Khafagy, K., Sorini, C. & Chattopadhyay, A., “Effects of defects on ceramic matrix composite response: High-fidelity creep modeling”. Composite Structures*,* (in preparation).

Conferences

1. Khafagy, K., Venkatesan, K., Balusu, K., Datta, S. & Chattopadhyay, A., “Stochastic microstructural analysis of failure mechanisms in ceramic matrix composites using a high-fidelity multiscale framework”, *AIAA Science and Technology Forum and Exposition, January 11-15*, (2021), Nashville, TN, USA.
2. Khafagy, K. & Chattopadhyay, A., “Effects of as-received defects on ceramic matrix composites properties using high-fidelity microstructures with periodic boundary conditions”, *The American Society for Ceramics. September 19-22*, (2021), Tx, USA.

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