Multiscale Modeling of Functionally Graded Hybrid Composites and Joints

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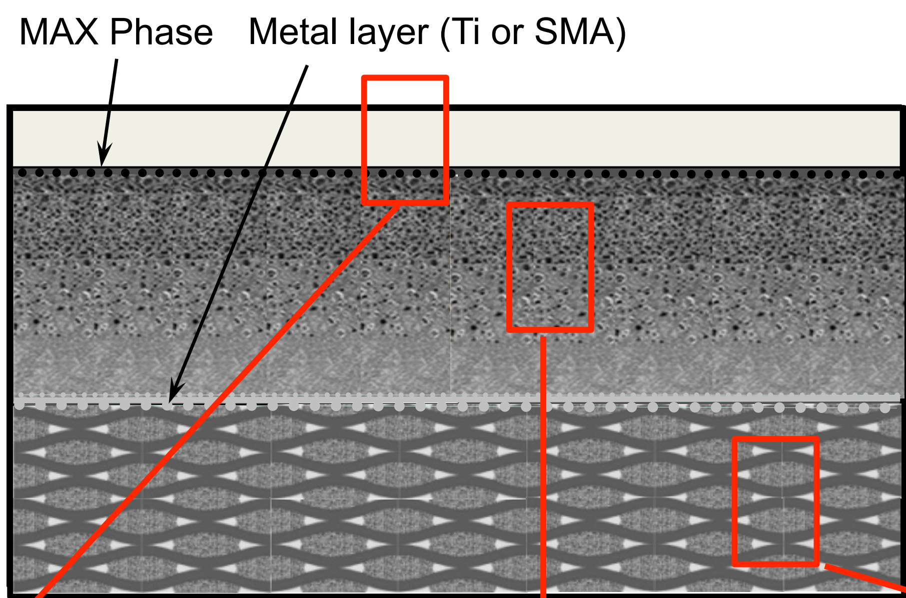
Functionally Graded Hybrid Composites (FGHCs) – The concept

Materials

Oxide ceramic

Functionally graded ceramic/ metal composite (**GCMeC**)

Polymer matrix composite (**PMC**)

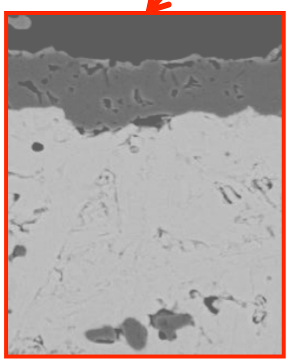


Function

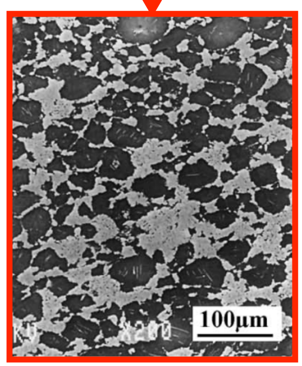
Thermal/Environmental Barrier Coating (Al_2O_3, ZrO_2, PS-ZrO_2)

Self-healing of Protective Coating
Gradual Change in Thermal Expansion
Thermal Management
Mechanical Damping
Compressive Stress on Ceramc

Load Bearing
Host Sensors
Damage Propagation Barrier



15 μm thick protective Al_2O_3 surface layer formed after 10,000 heating cycles of Ti_2AlC

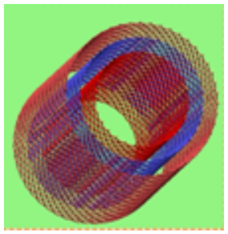


Ti_2AlC (light) + γTiAl (dark) as example of MAX phase composite

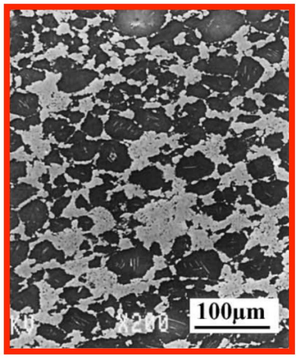
Actively Cooled PMC with microvascular cooling functionality and/or High Temperature PMCs with polyimide matrices

Wide Range of Scales

Fuzzy fiber



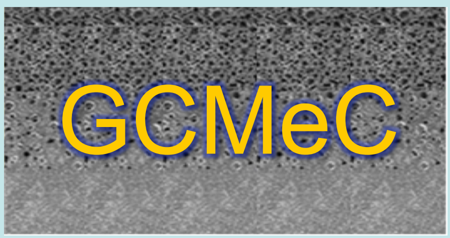
Seidel



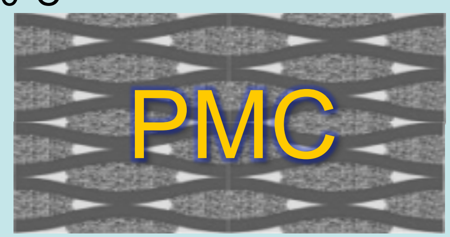
Gao
Geubelle
Lagoudas
Whitcomb

Cizmas

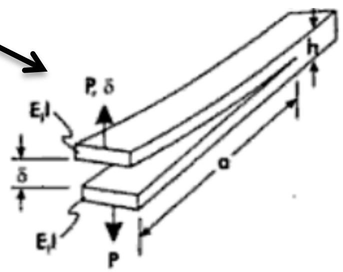
1000°C

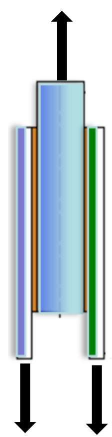


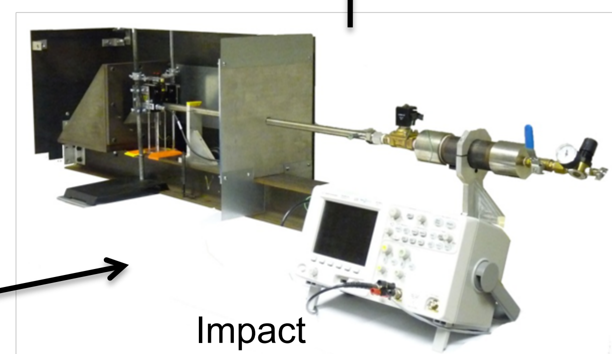
300-400°C



Optimize FGHC







Impact

Ochoa
Whitcomb

Reddy

Overview of Goals

- Predict performance of material and components fabricated from FGHC
- Develop strategies for joining parts
- Expedite mechanical and thermal design of functionally graded hybrid composite (FGHC)
- Define in-flight mechanical and thermal loads

Perspectives

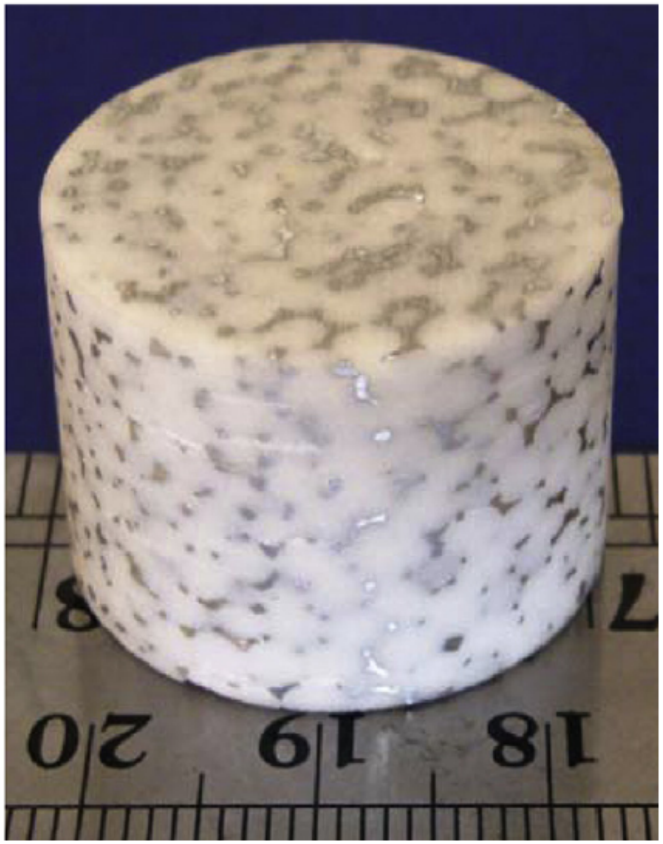
- Scales: molecular dynamics
  micromechanics
  mesomechanics
  specimens (e.g. DCB)
  components

- Material models: mechanical, thermal, electrical
  linear elastic
  viscoplastic
  progressive damage
  shape memory

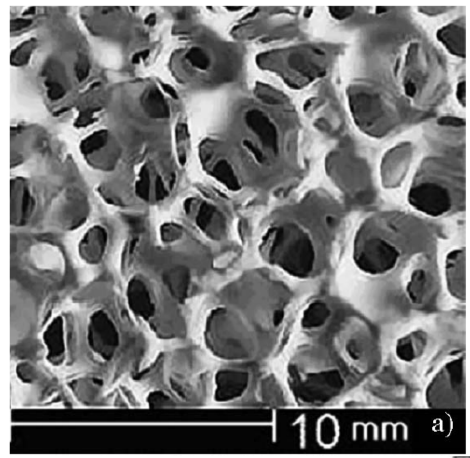
- Loads: steady-state mechanical and thermal
  transient mechanical and thermal
  impact
  aeroelastic

Modeling GCMeC as Interpenetrating Phase Composite

3-D Preform



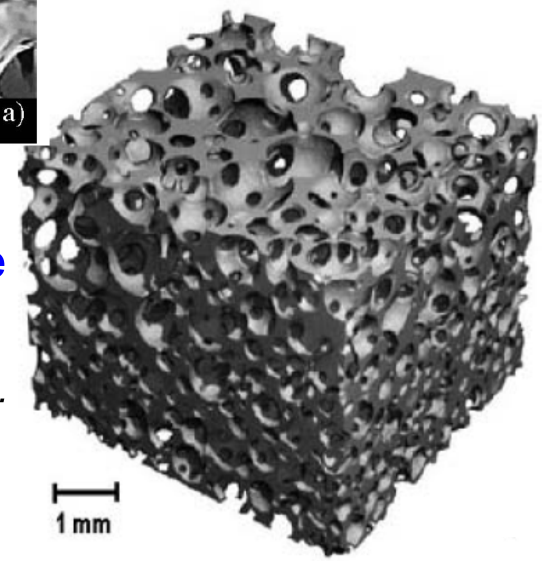
(Jhaver and Tippur, *MSE-A*, 2009)



SEM micrograph
of Al_2O_3 preform

Micro-CT scan image
of preform

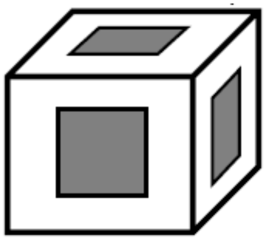
(Colombo & Hellmann, *Mat. Res. Innovat.*, 2002)



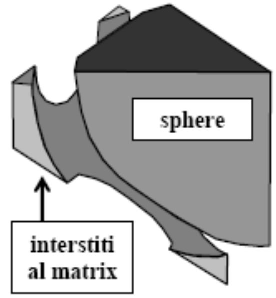
Preform as a random 3-D open-cell foam

Micromechanical Modeling of Interpenetrating Phase Composite (IPC)

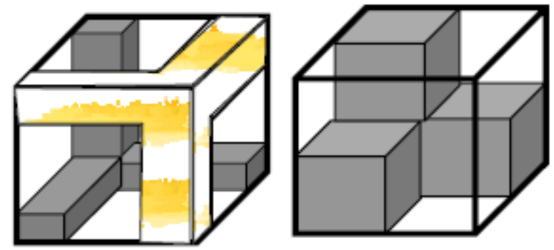
- **Unit cell-based models:** **unable to account for random features in IPCs**



3-D cubic unit cell model
(Daehn et al., 1996)



Triangular prism unit cell model
(Wegner and Gibson, 2000)



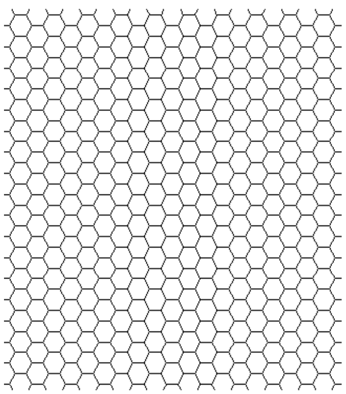
2- and 3-phase unit cell models
(Feng et al., 2003, 2004)

- **Proposed work**

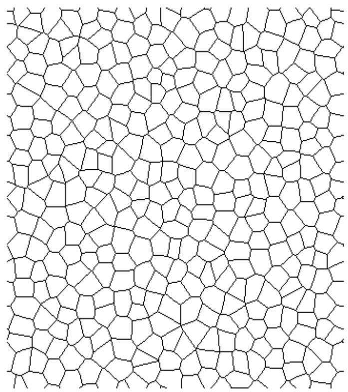
  - Extracting microstructural data from actual GCMeC using **X-ray micro-CT**
  - Developing new unit cell models incorporating microstructural features of GCMeC
  - Developing random cell models including **hundreds of cells** that are **irregular** in cell shape, **non-uniform** in strut cross section area, and **different in porosity** by using the **Voronoi tessellation** technique and the **finite element method** with **periodic** B.C.s
  - Performing **parametric studies** of composites containing various candidate constituent materials and different topological features to identify an **optimal design** of GCMeC

Random Cell Model

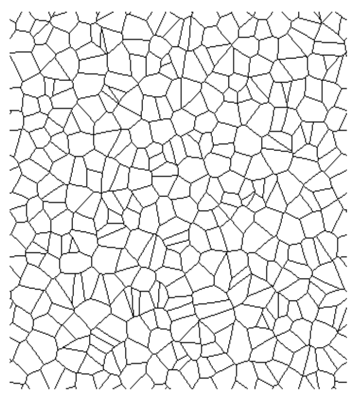
- **Periodic random models – Preliminary Work**
  - Start with **reference model**: structure with regular cell shapes and uniform SCSAs
  - Construct from a set of **periodically located seeds** using **Voronoi tessellation** technique



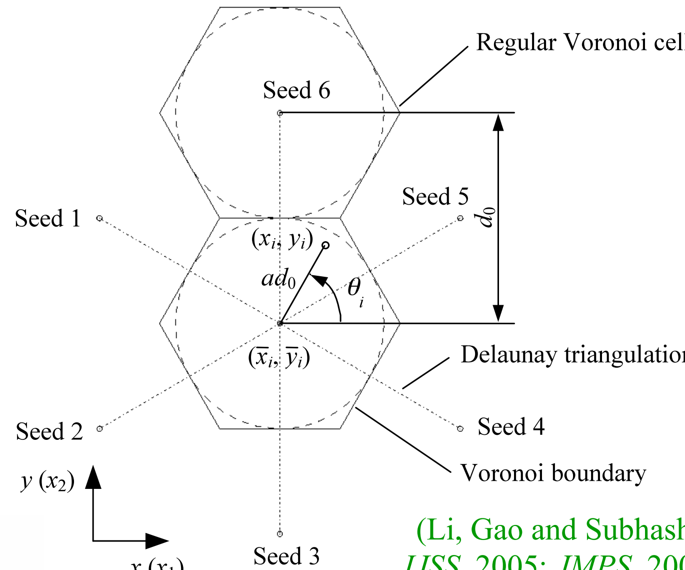
Reference (a = 0)



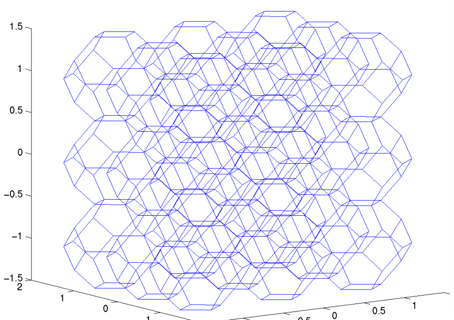
Random (a = 0.5)



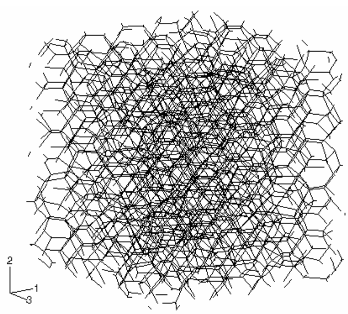
Random (a = 1.0)



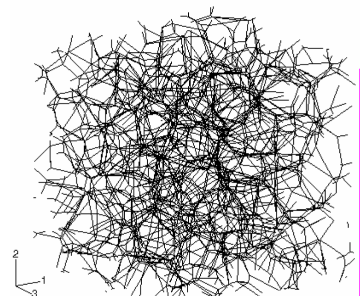
(Li, Gao and Subhash, *IJSS*, 2005; *JMPS*, 2006)



$a = 0$



$a = 0.1$



$a = 0.5$

Coordinate perturbations of a seed

$$x_i = \bar{x}_i + a(d_0 \cos\theta_i)\varphi_i,$$

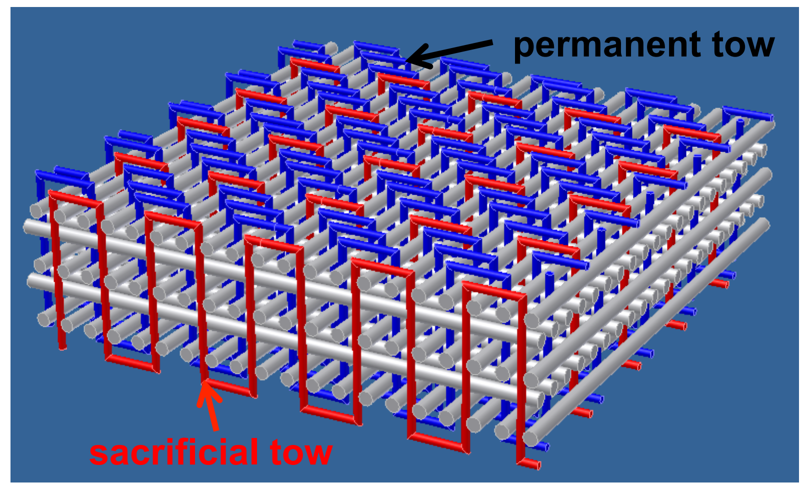
$$y_i = \bar{y}_i + a(d_0 \sin\theta_i)\varphi_i,$$

$$\theta_i \in [0, 2\pi], \qquad \varphi_i \in [-1, 1],$$

$a \in [0,1]$ **cell shape irregularity amplitude**

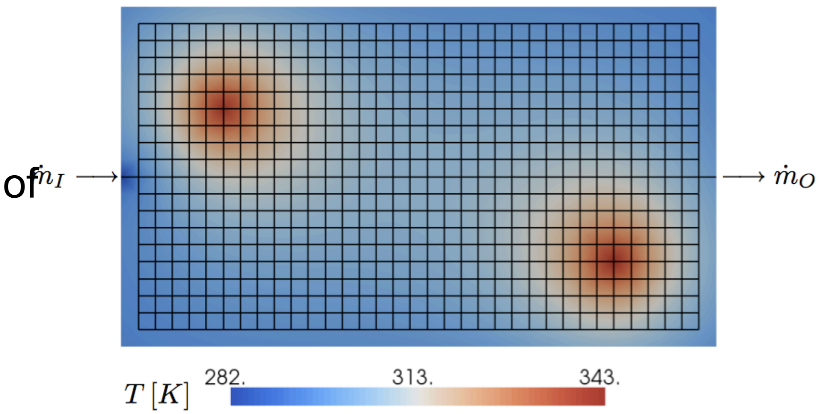
Actively Cooled 3D Woven PMC

- Computational design of microvascular networks embedded in actively cooled 2D and 3D woven PMC
- Prediction of homogenized thermo-mechanical response of composite with embedded cooling network
- Technical challenges
  - Accurate representation of composite microstructure
  - Definition of network template compatible with microstructure and manufacturing constraints
  - Problem size
  - Validation with thermal and constitutive/failure assessments (White and Sottos)
  - Multiscale thermal and structural modeling of AC-PMC

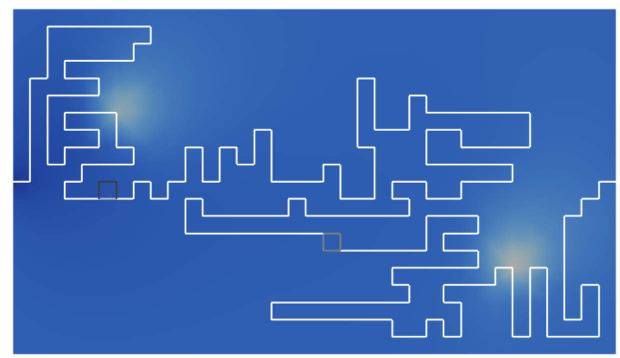


Related Work: Computational Design of Microvascular Polymer

- Multiphysics modeling and optimization of 2D microvascular networks for actively cooled polymers
  - **Generalized finite element** (GFEM) modeling of thermal response of polymer components with embedded microvascular network
  - Multi-objective/constraint NSGA-II **genetic algorithm** for **discrete optimization** problem with very large design space

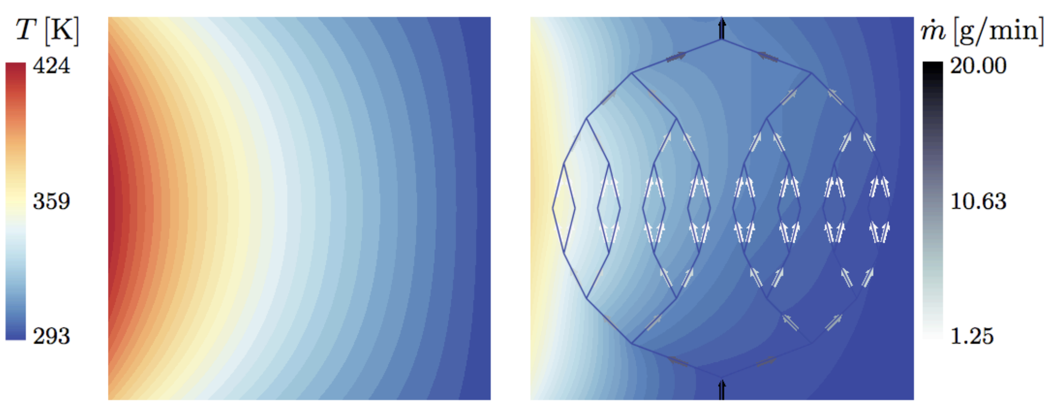


Thermal response in absence of network and defining template



Network for optimal thermal response

Active cooling of polymer component with two localized heat sources



Without network

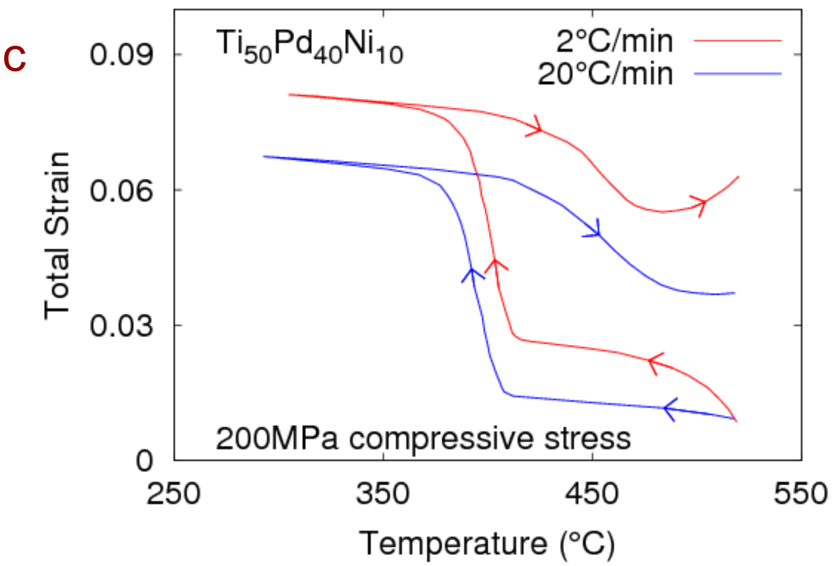
With embedded network

GFEM modeling of thermal response of epoxy with 4-level branched cooling network

Viscoplastic Behavior of High-Temperature Active Layers

Use shape memory effect to absorb energy and induce compressive stresses in ceramic

- High temperature=> viscoplastic response becomes an important issue for the metallic constituent
- Creep is directly coupled with the transformation behavior of high-temperature SMAs

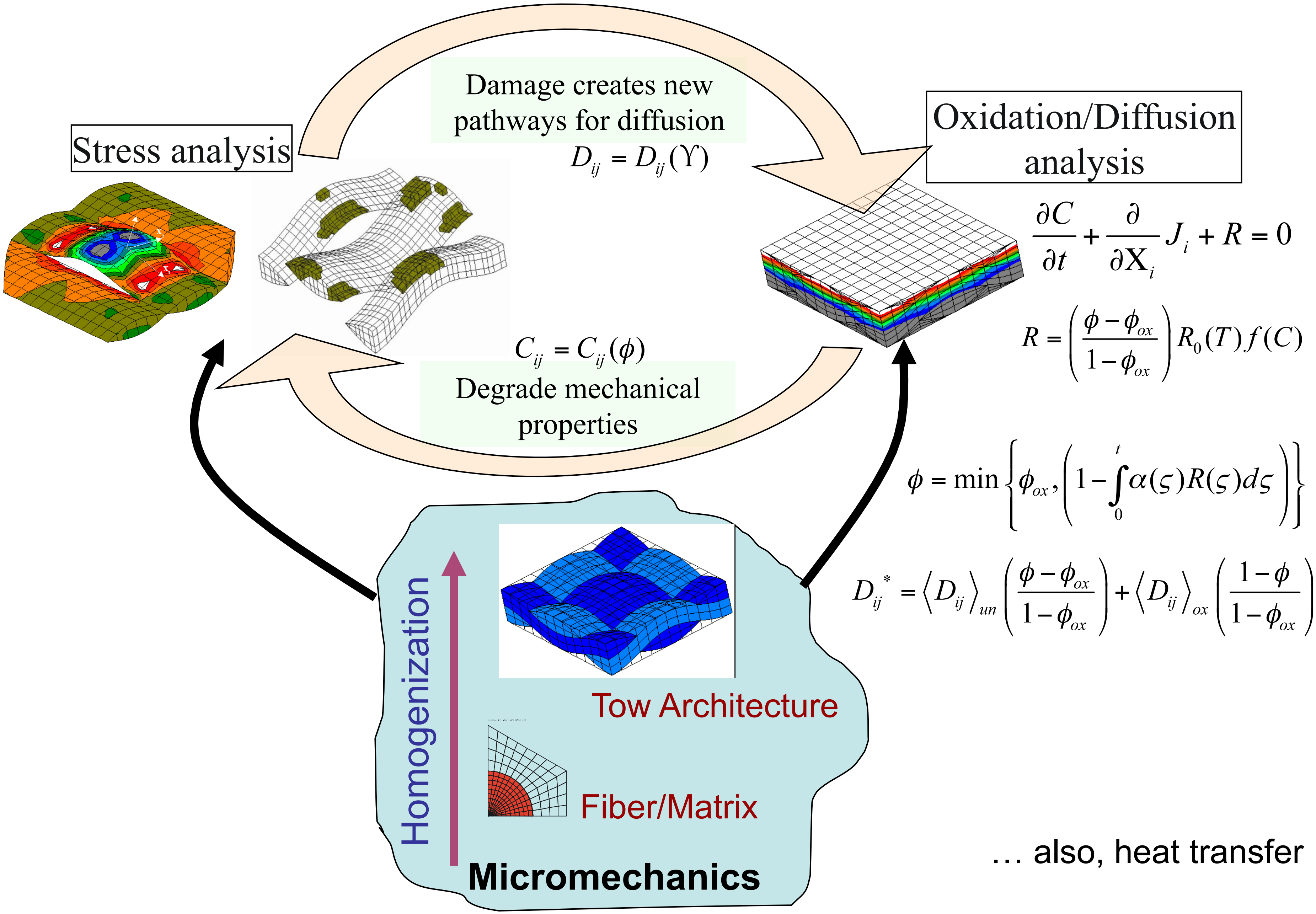


- Characterize overall creep behavior of GCMeC
- Optimize microstructure with respect to its inelastic performance
- Obtain effective creep properties by extending multiscale homogenization techniques

Multiscale Analysis of Progressive Damage in FGHC

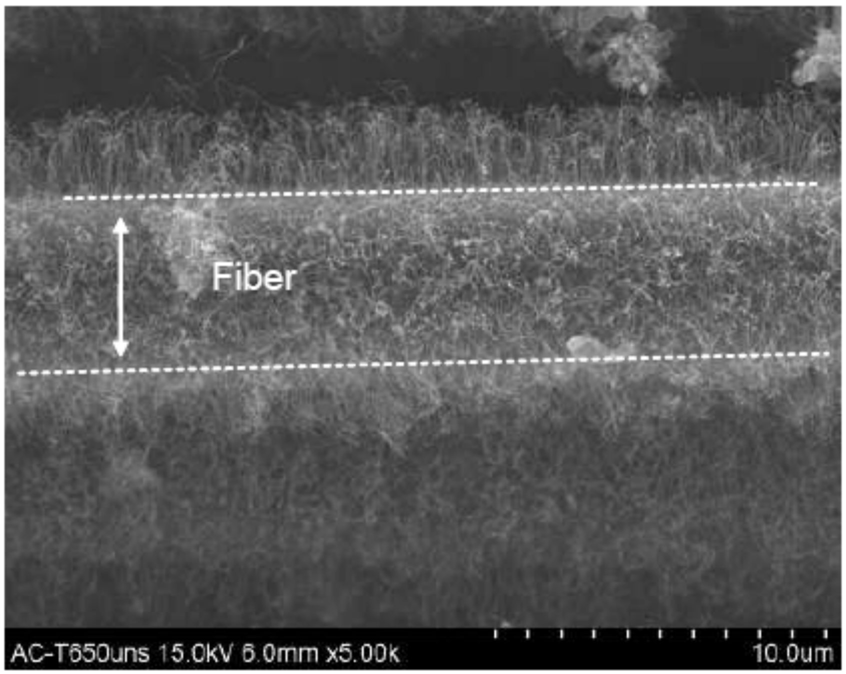
- Damage mechanics algorithms (improve accuracy)
- Expedite analysis to facilitate parametric study
  - Algorithms to reduce computational cost (human and cpu time & memory)
    - ✓ Finite elements w/ internal microstructure
    - ✓ Alternative homogenization schemes
    - ✓ GFEM
  - Parallel computation
- Configurations
  - Micro (e.g. fiber/matrix)
  - Meso (e.g. textile unit cell)
  - Macro (e.g. DCB)

Multi-scale/Multi-field Modeling of Damage



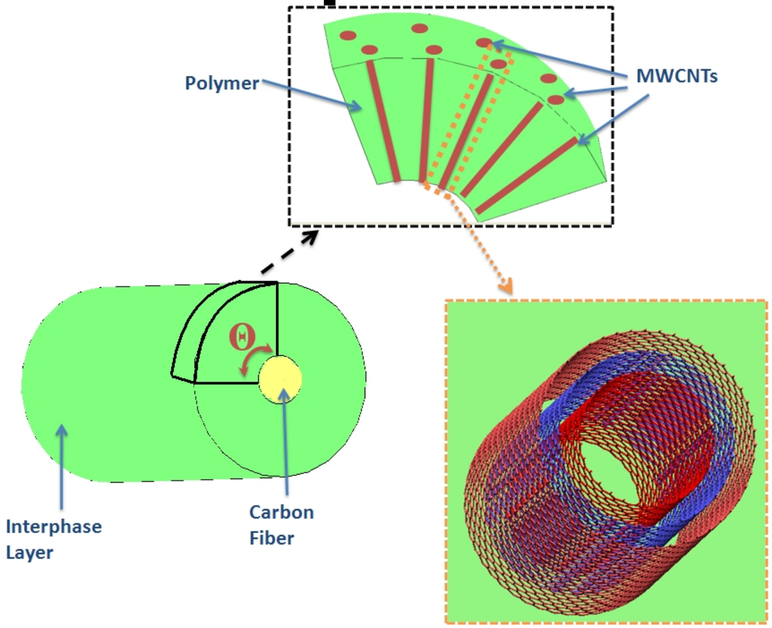
Fuzzy Fibers for Structural Health Monitoring

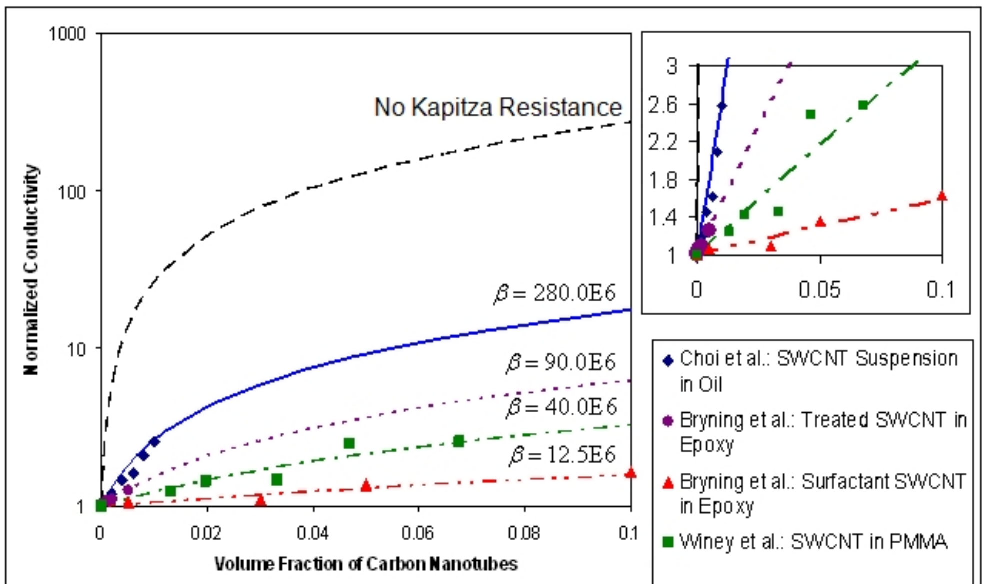
'Fuzzy' fibers: SiC fiber core with carbon nanotubes grown radially along fiber length



- Develop multiscale model correlating changes in electromechanical properties with damage evolution within nanocomposite interphase of fuzzy fiber under quasi-static mechanical and thermal cycling
- Explore design space for fuzzy fibers as SHM sensors through correlation of fuzzy fiber design parameters with sensing properties
- Integrate multiscale model for fuzzy fibers with higher length scale models for application in full multiscale model for FGHC

Nanocomposite-based SHM: Key Challenges





Influence of interfacial thermal resistance on nanocomposite themral conductivity

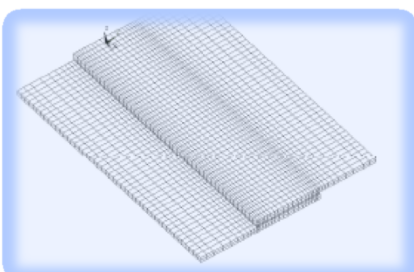
- Adaptive multiscale computational micromechanics tools which integrate a) molecular dynamics b) finite element analysis, and c) homogenization techniques
- CNT-Polymer mechanical and thermal interface effects into continuum level models (inelastic cohesive zone models)
- Incorporation of nanoscale effects of electron hopping and interfacial thermal resistance
- Incorporation of polymer damage evolution model in nanocomposite interphase
- Incorporation of electromechanical properties of CNTs and its influence on fuzzy fiber SHM capabilities

Integrity of Interfaces

Assist the design of joints tailored for multiple interfaces present in multilayered system

- **MAX - Hybrid Composite**
- **Metal - Laminates (TiGr)**
- **PMC – Metal (Ti)**

✓ FEA models based on the microscopy and micro-CT observations of functionally gradient interfaces to integrate geometric and material heterogeneity



✓ Mechanical and thermal compatibility and integrity of interfaces addressed through thermo-oxidative response to gain insight to damage mechanisms

Aero-thermo-elasticity

- Predict aero-thermoelastic response using a high-fidelity, non-linear aeroelastic solver for two configurations
  - Canonical double-wedged wing
  - Typical hypersonic vehicle
- Evaluate thermal effects on AE response including material degradation
- Assess effect of elastic deformation on aerodynamic heating
- Evaluate impact of inertial effects in pre-flutter aero-thermoelastic analysis

- Augment in-house AE solver that uses a RANS flow model and FEM structural solver (including thermal stresses and material degradation)
- Include heat transfer in flow/structure coupling

Summary

- A wide range of
  - Material systems
  - Numerical techniques
  - Length and time scales
- Expected outcome: guiding the design of functionally graded hybrid composite for hypersonic vehicle application