Image analysis, synthesis and image-based modeling of ceramic-matrix composites

Gerard L. Vignoles
University of Bordeaux, France, vinhola@lcts.u-bordeaux.fr

Follow this and additional works at: http://dc.engconfintl.org/acmc

Part of the Engineering Commons

Recommended Citation

This Abstract and Presentation is brought to you for free and open access by the Proceedings at ECI Digital Archives. It has been accepted for inclusion in Advanced Ceramic Matrix Composites: Science and Technology of Materials, Design, Applications, Performance and Integration by an authorized administrator of ECI Digital Archives. For more information, please contact franco@beypress.com.
IMAGE ANALYSIS, SYNTHESIS AND IMAGE-BASED MODELING OF CERAMIC-MATRIX COMPOSITES

… some research by the
Laboratory of Thermostructural Composites
UMR 5801
CNRS-Safran-CEA-Université de Bordeaux

Gerard L. Vignoles

The ECI CMC Conference, Santa Fe, NM, Nov. 2017
Laboratory for ThermoStructural Composites

Founder: Pr. Roger Naslain (1988)

Joint research unit UMR5801 created in 1988, 4 partners:

- Centre National de la Recherche Scientifique (CNRS)
- Université de Bordeaux (UBx) - Science & Technology
- Safran
- Atomic & Alternative Energies Agency (CEA, 1999)
Competences at LCTS

Processing
- Matrix
  - Liquid route
  - Gas route
- Fiber
  - Interphase interface
  - Surface treatment
  - Pyrolysis

Characterization
- Composition
- Structure
- Texture
- Morphology
- SEM, E-SEM, TEM
- XRD
- XRCT, image processing

Testing
- Mechanical
- Thermal
- Oxidation
- Constituents
- Bulk material
  - High-temp fatigue
  - HP/HT
  - Corrosion
  - Uncoupled solicitations
- Nano-indentation
  - Tests on filament/minicomposite
  - Thermokinetics

Modeling & simulation
- Process
  - Full model
  - Micro-meso-macro models
- Material
  - Multi-scale Numerical methods
Outline

- Context
- Image analysis & synthesis
- Modelling Gas-phase Infiltration of Ceramic Matrices
- Modelling evolution under high-T oxidation
- Modelling mechanical behavior
- Conclusion & perspectives
Part 1

CONTEXT
CMCs in new-generation aircraft engines

**Silicon & boron carbide based multilayer matrix**

**Carbon/ SiC fibers**

**Woven 3D architecture**

**Aircraft engine parts**

Ceramics → lighter, more refractory → energy savings, less pollution

November 6, 2017  G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Ceramic Matrix Composites (CMCs)

- **Ceramic fibers**: high modulus & strength, even at high T
- **Ceramic Matrices**: Stiff & strong, Compatible with fibres
- All components are brittle! But matrix **multicracking** occurs
- **Interphases**: crack **deviators**
- **Cracks = paths for** corrosion
- **Protective layers** inserted in matrix

G. Camus, 1996

Déformation > 1%
Motivations, objectives

- High standard materials, costly fabrication
- Need to guarantee performances
- Need to optimize production without increasing, or lowering costs

→ Pertinence of numerical simulation & of validated modeling

→ Handling NUMERICAL / VIRTUAL materials & processes
Before going virtual … be actual!

- Try & describe the material *as it is*
  - Morphological analysis
  - «Non-destructive» characterization
- Extract descriptors to feed an «*in silico*» material synthesis
- *Validate experimentally* the behavior simulated from constituents and their arrangement
- Varying descriptors enables *optimizing* virtual materials
# Virtual material strategy

<table>
<thead>
<tr>
<th>Actual material</th>
<th>Numerical representation</th>
<th>Virtual material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Structural characterization</td>
<td>Morphological analysis</td>
<td>Design workshop</td>
</tr>
<tr>
<td>Properties of individual constituents</td>
<td>Representation of structure</td>
<td></td>
</tr>
<tr>
<td>Characterization of material behavior</td>
<td>Image-based modeling (featuring change of scale)</td>
<td></td>
</tr>
</tbody>
</table>

- **Validation**
- **Effective macro behavior**
- **Prediction**
- **Simulated macro behavior**

---

November 6, 2017  G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Virtual process strategy

<table>
<thead>
<tr>
<th>Actual process</th>
<th>Numerical representation</th>
<th>Virtual process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry reactor, substrate, etc…</td>
<td>Morphological analysis</td>
<td>Design workshop</td>
</tr>
<tr>
<td>Characterization flow reactions, …</td>
<td>Representation of structure</td>
<td></td>
</tr>
<tr>
<td>Large-scale characterization (whole part)</td>
<td>Aerothermal &amp; physicochemical computations (featuring change of scale)</td>
<td></td>
</tr>
<tr>
<td>Validation</td>
<td>Effective macro behavior</td>
<td>Prediction</td>
</tr>
<tr>
<td></td>
<td>Simulated macro behavior</td>
<td></td>
</tr>
</tbody>
</table>

November 6, 2017  G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Modeling activities

- Infiltration modeling
- Self-healing modeling
- Mechanical modeling
- CMC imaging & analysis
Part 2

IMAGE ANALYSIS & SYNTHESIS
Detecting orientations in images

\[
\mathbf{T} = \begin{pmatrix}
\left(\frac{\partial I}{\partial x}\right)^2 & \frac{\partial I}{\partial x} \frac{\partial I}{\partial y} & \frac{\partial I}{\partial x} \frac{\partial I}{\partial z} \\
\frac{\partial I}{\partial x} \frac{\partial I}{\partial y} & \left(\frac{\partial I}{\partial y}\right)^2 & \frac{\partial I}{\partial y} \frac{\partial I}{\partial z} \\
\frac{\partial I}{\partial x} \frac{\partial I}{\partial z} & \frac{\partial I}{\partial y} \frac{\partial I}{\partial z} & \left(\frac{\partial I}{\partial z}\right)^2
\end{pmatrix}
\]

Image structure tensor

\[= P^{-1}.\text{diag}(T).P\]

\(\mu\text{CT}\)

☺ Fast & automatic

☺ Image-based : realistic

Yarn direction

2D example

Grayscale level gradient

Notion of yarn

Highly dependent on CT scan quality
Yarn retrieval software : GenDir

New method under development : image-guided relaxation
⇒ Minimal manual operation
⇒ More robust
⇒ Avoids interpenetrations
Macro-wire virtual weaving: GenFil

3D weaving:
Geometric model,
with appropriate topology

Intermediate model made of
macro-wires subject to mechanical equilibrium

Synthesis of fibers in a yarn

Uses an « object dynamics » algorithm (Verlet) for a 2D slice
+ Continuation in 3D

C. Chapoullié, PhD diss.
U. Bordeaux (2015)
Image processing: summary & outlook

Numerical tools & strategy

• Orientation detection is a key tool
• 2-scale work
• Efficient software tools, now transferred to industry
• The next question is: how to transfer to numerical simulations?

Outlook

• Improving the robustness & CPU/memory demand of the methods
MODELLING OF GAS-PHASE INFILTRATION OF CERAMIC MATRICES
Fabrication of CMCs

3D fiber weaving

Preform

Preceramic Slurry Impregnation & Pyrolysis (SIP)

Chemical vapor Infiltration (CVI)
Fibers + SIP matrix

How “infiltrable” is this??
Modeling strategy

• Acquisition & processing of **tomographic images**
• Development of two software “porous media” codes: **fiber scale** & **composite scale**
• **Connection** of the two codes through effective laws

2-scale modeling strategy

- Splitting into sub-volumes
- Computation of properties in each sub-volume
- Identification of porosity & fiber orientation
- Injection of laws
- Infiltration simulation over whole width of the composite part

Laws: \( \text{Props} = f(\text{poro}) + \text{statistics of dispersion} \)
Investigated preforms

Images acquired by X-ray CMT:
ESRF ID19 line

Two resolutions for acquisition:
1.4 μm/pixel and 5 μm/pixel

SiC 3D woven fabrics with
Pre-deposited SIP matrix

November 6, 2017   G. L. Vignoles   ECI CMC Conference, Santa Fe, NM
Two distinct fibrous arrangements

Preform M1

Preform M2

Frequency

Pore volume fraction (-)

Frequency

Internal surface area (pix\(^{-1}\))

November 6, 2017    G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Fiber-scale infiltration modeling: DMC

« Kinetic » Random walk w/ reaction and surface growth

1. Start of time process
   - Random position
   - Random direction
   - Isotropic distribution

2. Binary collision
   - Time until next collision
   - Random direction
   - Isotropic distribution

3. Wall collision without reaction
   - Random direction
   - Knudsen’s cosine law

4. Wall collision with reaction

Random position and direction
Binary collision
Voxel borders
Wall collision
End of time process


November 6, 2017  G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Large-scale infiltration modeling: LIRWa

- Itô-Taylor random walks

Diffusive step: random direction with anisotropic Gaussian distribution following $D$

Diffusion tensor $D$ computed in each voxel from greyscale value (density) and local fiber orientation

Adective step following $\text{div} D$ (heterogeneity)

« Russian roulette » for deposition reaction

Gas diffusion – intermediate regime

\[ \eta = \frac{\eta^{bin} + Kn \eta^{Kn}}{1 + Kn} \]

Intermediate regime tortuositities
(Kn = 0.3)
Incorporating dispersion

Injection of the observed statistical data

Computation of the ratio between actual value and fitted law value

At large scale: theoretical value is biased by a random drawing with injected cumulative frequency

Validation: distributions from actual micro scale and computed macro scale are equivalent
Simulation of infiltration

Integration of the effective laws + dispersion in macroscale solver

Downgrading the macroscale tomographs resolution \(\rightarrow\) computational time savings

Infiltration simulations for different values of the heterogeneous reaction constant

Comparison of macroscopic properties of each preform

Preform M1

Preform M2

Through-the-thickness effective diffusion coefficient (m².s⁻¹)

- M1 khet = 0.1 m/s
- M1 khet = 0.05 m/s
- M1 khet = 0.01 m/s
- M1 khet = 0.005 m/s
- M2 khet = 0.1 m/s
- M2 khet = 0.05 m/s
- M2 khet = 0.01 m/s
- M2 khet = 0.005 m/s

November 6, 2017  G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Discussion

**M2 has a better « infiltrability » than M1**

Whatever the processing conditions, **preform M1 gets plugged faster** than preform M2.

The microscale conclusions are **verified** at the composite scale.

**Identification of the parameters controlling infiltrability → An efficient engineering tool**
Modeling Chemical Vapor Infiltration in a virtual material

Matrix thickness profile
CVI modeling : Summary

Numerical tools & strategy

• Two distinct numerical methods, specific to micro & macro scales, were chained together

• Work on 3D images (X-ray CMT scans, or virtual)

Comparison of the infiltrability of SiC_f/SiC_{SIP} preforms

• Comparison of effective diffusivity, reactivity and microscale geometrical parameters

• Evidence of their effect on the macroscale infiltrability of these preforms

Insertion in a virtual material toolbox

• Computation at various scales

• A design tool from weaving to the final matrix

• Transferred to the industry
MODELLING OXIDATION AND SELF-HEALING
Problem assumptions

Transverse crack image-based modeling:
- Crack width is a function of 2D space
- Diffusion of oxygen as gas and/or dissolved species in liquid
- Liquid height is a function of space
- Evolution equation for interphase consumed height
- Liquid spreading
- Volatilization is not (yet) accounted for

Mechanical behavior:
- Weibull distribution
- SCG law \( \Rightarrow \) strength decrease
Lifetime computation algorithm

- Plug formation
- Crack sealed?
  - Yes: Calculate the oxygen rate around the fibers
  - Yes: Oxide spreading
- Fiber breakage?
  - Yes: Compute stress
  - Yes: Calculate the crack height
  - Yes: Wider opening?
- Oxidation process
- Mechanical stress
Resolution domain: minicomposite
Fine mesh for physico-chemistry
Coarse mesh for mechanics
Variable crack width
O$_2$ concentration (mol.m$^{-3}$) vs. Time (hours)
Sealing behavior

Sealing period

Plug formation

F is reached by the liquid oxide

Time (hours)

Cumulative $O_2$ concentration (mol.m$^{-3}$.s)

$t = 0.2$ h  

$t = 1$ h  

$t = 2$ h  

$t = 5$ h  

November 6, 2017  

G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Fiber failure & local reloading
Meso-model of oxidation, healing, partial fiber breakage and re-healing

Crack oxidation and sealing
November 6, 2017

Breakage: crack reopening

Oxidation restarts
Progressive failure of the bundle

Time (hours)

Number of broken fibers

G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
SH-CMC simulation: Summary

Numerical tools & strategy

• Image-based approach

• Multiphysics code

• Gives convincing scenarii for bundle weakening & failure

Outlook

• Perform a statistical study

• Extension to longitudinal cracks

• Integration in crack networks

New funding obtained!
MODELLING OF MECHANICAL BEHAVIOR
Non-linear mechanics due to multicracking:
- Localization of stress concentrations
- Introduction of cracks in FE meshes
- How to get a good FE mesh, by the way?
Yarn-scale FE mesh generation


μ-CT scan

Manual contouring on 2 transverse slices

Orientation detection & segmentation

Marching-cube & simplification + Volume meshing
Fiber-scale FE mesh generation & computations

Micrographs

Segmentation of fibers & matrix

2D Meshing

Numerical homogenization

\[ \langle \epsilon \rangle = \frac{1}{V_{\Omega}} \int_{\Omega} \epsilon \, dV, \quad \langle \sigma \rangle = \frac{1}{V_{\Omega}} \int_{\Omega} \sigma \, dV \]

\[ \langle \sigma \rangle = C^{\text{app}} : \langle \epsilon \rangle \]

The transverse isotropic properties are transferred to yarns

\[
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\sqrt{2} \epsilon_{33} \\
\sqrt{2} \epsilon_{13} \\
\sqrt{2} \epsilon_{12}
\end{pmatrix}
= 
\begin{pmatrix}
\frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & -\frac{\nu_{13}}{E_1} & 0 & 0 & 0 \\
-\frac{\nu_{12}}{E_2} & \frac{1}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\
\frac{\nu_{13}}{E_3} & -\frac{\nu_{23}}{E_3} & \frac{1}{E_3} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2G_{23}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2G_{13}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{12}}
\end{pmatrix}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sqrt{2} \sigma_{23} \\
\sqrt{2} \sigma_{13} \\
\sqrt{2} \sigma_{12}
\end{pmatrix}
\]
Tensile test under $\mu$-CT


Hydraulic load
5000N

Air cooling

Joule heating

X-ray source
(GE Vtom X, Placamat)

SiC/SiC MI samples
Section : 2x3 mm$^2$
Gauge length: 10 mm
In-situ testing


ID19 beamline ESRF
Resolution : 1 µm
Crack detection by image analysis


Procedure:

i. *Scaling factor*: 2
ii. *RBM correction* (Avizo ®)
iii. *Difference fields*
iv. *Morphological filters*
v. *Manual control*

- Cracks from surface, perpendicular to tensile load
- Initiation & propagation in pre-damaged zones

Procedure:

Retrieval of boundary conditions by DVC


(a) Normalized DVC displacement components evaluated in *

(b) Normalized DVC displacement components evaluated in **

Actual strain
Elastic computations


Cracks & overloads coincide

November 6, 2017   G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Multi-scale damage modeling

Micro cells

Cohesive interface, brittle matrix

Mesoscale damage computation

Transposition of stiffness abatement

... IN PROGRESS ...
A-FEM method


Mechanics: Summary & Outlook

Numerical tools & strategy
- From images to FE meshes
- Multi-scale strategy
- Experimental verification vs. μ-CT:
  - Role of DVC in crack detection & BC retrieval
  - Cracks match overloaded areas (yarns crossings)

Outlook
- FE meshing procedure development still under way
- Failure mechanics under way …
General conclusion

- Multiscale /multiphysics approaches
- Dialog between experiments & modeling
- Multidisciplinary work:
  - Structural characterization (image acquisition; properties)
  - Image processing (analysis; synthesis)
  - Physico-chemical (« multi-physics ») modeling
  - Numerical tools (meshes, solvers, etc …)
- A broad field of possibilities: every material, every application brings its « own » physico-chemistry
- From basic science to application and innovation
Acknowledgements

Permanent staff

G. Couégnat
O. Caty
F. Rebillat
G. Camus
E. Martín
C. Descamps
A. Mouret
S. Denneulin
T. Vandellos

PhD, PD and MS students

H. Ayadi
C. Saurat
T. Haurat
C. Mulat
W. Ros
C. Chapoullié
V. Dréan
G. Perrot
L. Halé
S. Essongue
V. Mazars
J. Bénézech

November 6, 2017   G. L. Vignoles – ECI CMC Conference, Santa Fe, NM
Acknowledgements

Collaboration

C. Germain
J.-P. Da Costa
M. Donias

M. Ricchiuto

S. Roux
A. Bouterf

Funding

New!
¡Gracias por su atención!
¿Preguntas?
Workshop announcement

**Bulk Carbon Materials** (composites, fibers, films, foams, porous carbons, etc.):

**Relationships between processing conditions and the resulting structure, texture, and properties**

a.k.a. “the 3rd PyroMaN workshop”

Madrid, Spain       June 29-30, 2018

vinhola@lcts.u-bordeaux.fr
monthioux@cemes.fr