MATERIAL CHARACTERIZATION WITH REPRESENTATIVE VOLUME SIMULATIONS OF WOVEN POLYMER MATRIX COMPOSITES

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1 Introduction

A distribution of constitutive responses is obtained using material and geometric measurements with representative volume elements (RVE). The geometrically accurate RVEs are used for detailed stress concentration and damage initiation and propagation analysis. Finite element modeling of the meso-structure over the distribution of characterizing measurements is automated and various boundary conditions are applied. Plain and harness weave composites are implemented. Continuum yarn damage, inter-yarn debonding and an elastic-plastic matrix are combined with known materials and geometries in order to estimate the macroscopic response as characterized by a set of orthotropic material parameters. Damage mechanics and coupling effects are investigated and a macroscopic material model is demonstrated and discussed. Prediction of the elastic, damage, and failure behavior of woven composites will aid in macroscopic constitutive characterization for modeling and optimizing advanced composite systems.

Macroscopic constitutive relations for composite damage evolution analysis are abundant in literature [1-6]. Fully characterizing even the most common place damage evolution and failure models requires difficult to implement experiments. In addition to elastic characterization, an approach is presented to obtain estimates of the damage/plastic initiation/evolution parameters.

The constituent (fiber, matrix) properties are often given in literature, manufacturing specifications or by a few simple tests. Validating/calibrating experiments are then used in conjunction with geometrically accurate micro/mesomechanical simulations. Additional loading conditions are then applied to the numerical model in order to further characterize the macroscopic response of the material.

2 Background and Motivation

While proper material characterization requires a great deal of experiments, often preliminary scoping and design requires only broad statistical bounds of the material parameters. Thus, the presented micro/mesomechanical material characterization procedures are not intended to replace experiments, but rather supplement the often expensive and difficult to obtain data required for even the most basic material scoping and initial design processes.

3 Materials, processing, and experimental methods

In order to validate finite element simulations, a series of quasi-static tensile experiments have been performed. In addition, edge and surface microscopy images have been investigated in order to accurately depict fiber bundle morphology and damage nucleation and growth behavior.

3.1 Materials

The glass fiber reinforced polymer (GFRP) material used for this investigation is a thermosetting polymer prepreg system with a total fiber volume fraction of approximately 48%. The fiber architecture is an eight-harness satin weave composed of E-glass fibers of 6 µm in diameter. A
representative unit cell of a post-mortem fractured surface for this architecture is shown in Fig. 1.

![Fig. 1. GFRP 8-harness satin weave fiber surface with a unit cell illustrated. Warp face is shown with the warp direction vertically oriented.](image)

### 3.2 Specimen Processing

Prepreg laminates have been hand laid from individual plies cut using a 4-axis CNC flatbed cutter. Panels (250 mm x 300 mm) composed of 6 plies have been laid up in a symmetric stack sequence with the warp face of each ply facing out away from the mid-thickness plane, and the warp direction oriented along the tensile loading direction. Panels were vacuum bagged and autoclave cured according to the manufacturer’s recommendations. Beveled end tabs were then secondarily bonded to consolidated panels and specimens were cut using a wet saw equipped with a diamond embedded blade. Resulting specimen geometry can be seen in Fig. 2, with the warp fiber direction being collinear with the specimen length.

![Fig. 2. Tensile testing specimen geometry](image)

### 3.3 Testing Procedure

Edge and surface optical microscopy has been performed in order to describe the geometric quantities and spatial distribution necessary to have accuracy in simulation efforts. Monotonic tensile testing in displacement control has then been performed at a displacement rate of 3 mm/min. Strain gage-based extensometers have been utilized to directly measure the axial and transverse strains. The gage lengths for the axial and transverse strain determination were 25.4 mm and 18.5 mm, respectively. Specimens were loaded to failure with load and strain data continually recorded at 10 Hz. Post mortem microscopy was then performed on specimen edges as well as the surfaces in order to correlate with model predictions.

### 3.4 Experimental Results

Edge and surface microscopy images have allowed the direct measurements of tow width, height, spacing and undulation frequency. The resulting morphology has been directly used for modeling input to reconstruct the geometry. A typical front edge micrograph can be seen in Fig. 3.

![Fig. 3. Front edge micrograph detailing warp fiber tow ends](image)

The in-plane unit cell geometry, as shown in Fig. 1 for a subsurface post-mortem ply, as well as from the top surface of a cured part in Fig. 4, give an idea of the fiber tow packing density. From these images, the average warp and weft yarn count is 23/cm and 22/cm, respectively.
When a laminate with various fiber direction angles is loaded in tension, the respective failure of the constituent plies occurs successively in the increasing order of strength [7]. For this particular 8-harness satin weave loaded in tension along the warp fibers, the weft fibers are oriented at 90 degrees to the loading direction. This loading will give rise to transverse cracking within the weft tows. Modulus decreases by approximately 46% at a strain of 0.36%. The modulus then increases by approximately 18% before decaying further as damage progresses. The knee behavior in the stress-strain relationship is shown in Fig 5.

4 Representative Volumes

The three dimensional geometry of a woven composite on the meso-scale for numerical analysis must be representative of the average true structure and contain certain approximations/assumptions that ease the meshing process. The mesh for simulation is contiguous. Overlapping yarn surfaces are self-similar and do not have a polymer layer of separation. For damage analysis, these are instead modeled with localization elements such as cohesive surfaces. Due to the conservation of fibers, the yarn cross-sectional area is more or less constant over the sweep path. Since the sweep cross-section naturally changes along the path, the latter criterion is not strictly achieved when yarns layup in a contiguous manner. Additionally, priority is given to experimentally determined dimensions and unknown dimensions and geometry will be determined from mesh-ability, geometric constraints and cross-section optimization.

4.1 Micro-mechanical fiber-matrix

The micromechanical model in [8, 9] is used to estimate elastic properties of the yarn as well as stress and strain concentration factors for use in micro to macro constituent damage evolution.

Applying the boundary conditions described in section 6.1 to calculate the homogenized stiffness tensor, the fiber strain concentration factor can be calculated as

$$A^f = \frac{1}{\sqrt{V_f}} \left[ C^f - C^m \right]^{-1} [\tilde{C} - C^m]$$

(1)

where $\tilde{C}$, $C^f$, and $C^m$ are the RVE homogenized, fiber and matrix stiffness tensors respectively. Similarly, from [1] the matrix strain concentration tensor is given as
$A^m = \frac{1}{V^m} [I - V^f A^f]$  \hspace{1cm} (2)

These tensors relate the volume average stresses and strains in the constituents to the total RVE values.

### 4.2 Plain Weave

The following equations and methodology describe the geometry of a plain weave representative volume element [10]. The equations are mapped in three dimensions as vertices, the vertices are joined with curves through spline interpolation and curves bound surfaces that enclose individual volumes. The yarn section contains four unique volumes that can be reflected, rotated and translated to generate a single RVE.

The following dimensions describe the plain weave yarn geometry:

- $a_w$: Warp peak to trough length
- $a_f$: Fill peak to trough length
- $w_w$: Warp yarn cross-sectional width
- $w_f$: Fill yarn cross-sectional width
- $h_w$: Warp yarn cross-sectional height
- $h_f$: Fill yarn cross-sectional height
- $b_w$: Warp sweep path amplitude
- $b_f$: Fill sweep path amplitude

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<diagram>
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**Fig. 7.** Plain weave RVE dimensions

All dimensions are measured as if corners are sharp. Geometry modifications, such as fillets or chamfers, can be completed in the final stage. For this write-up, warp yarns and fill yarns are oriented in the $x$ and $z$ directions respectively.

“Inner” refers to a shared curve. The inner warp path corresponds to the inner fill cross-section and the inner fill path corresponds to the inner warp cross-section for the overlapping volumes. The inner fill cross-section/warp path curve is given as:

$$y(x) = \left( h_f - \frac{h_w}{2} \right) \cos \left( \frac{\pi x}{a_w} \right) - \frac{h_w}{2} \hspace{1cm} (3)$$

The inner warp cross-section/fill path curve is given as:

$$y(z) = \left( \frac{h_f}{2} - h_w \right) \cos \left( \frac{\pi z}{a_f} \right) + \frac{h_f}{2} \hspace{1cm} (4)$$

The outer paths in the overlap section are simply a normal projection from the inner paths where the thickness along the normal is $h$. In order to preserve continuity, the mid paths vary linearly between the outer paths and the adjacent cross-section.

The outer cross-sections at the yarn symmetry planes (peak or trough of the wave) are given as

$$y(z) = b_w \cos(\pi p_w z) - b_w + h_f \hspace{1cm} (5)$$

for the warp yarn, and

$$y(x) = -b_f \cos(\pi p_f x) + b_f - h_w \hspace{1cm} (6)$$

for the fill yarn; where $p_w$ and $p_f$ are the periods for the warp and weft undulations respectively.

Multiple techniques are available to generate a curve that ensures mesh continuity and qualitative accuracy. For simplicity, up to 5th order polynomials are chosen to represent the edges of the fill and warp yarns ensuring all boundary conditions are satisfied.

The inner warp and fill mid cross-sections for the four volume element are determined by the fill and warp edges. The outer warp and fill mid cross-sections follow the constant mid thickness paths and are described by a similar formulation. A cross-section is generated by solving the periodic equations in the following form:
\begin{align}
y(z) &= C_{1w} \cos \frac{\pi z}{a_f} + C_{2w} \\
y(x) &= C_{1f} \cos \frac{\pi x}{a_w} + C_{2f}
\end{align}

(7) (8)

for warp and fill respectively.

Statistical distributions of meso-scale measurements [11] sampled with Latin hypercube are used to generate a series of RVEs. An in-house net surfacing algorithm is used to generate representative volumes. The plain weave pattern is the focus while 8 harness satin is demonstrated and discussed. Fig. 8 provides a plain weave RVE with medium to fine mesh.

Fig. 8. Plain weave RVE mesh

4.3 Satin Weave

The individual curves that make up the undulated portion of the harness weave meso-structure are similar to those in the plain weave with a few exceptions. First, the yarns in the 0/90 region typically can overlap, resulting in the appearance of a uniform cross-section. Therefore, a fill yarn approaching the undulation must originate from an overlapping solid and must undercut the corresponding warp yarn at undulation and vice versa. Second, for a first approximation, we generate a reduced RVE, with a single undulation and a proportional amount of non-undulating yarns compared to the complete RVE [12]. Figures 9 and 10 show the complete 8HS RVE and undulating region respectively.

Fig. 9. Finite element model of 8-harness satin weave

Fig. 10. Undulating region

5 Materials

An elastic-plastic material is chosen for the matrix, in which the material parameters are fit to available NEAT resin data. Interface damage (inter-yarn debonding and cracking at the yarn to matrix interface) is modeled with cohesive-surface elements and a mixed-mode [13] traction separation law with parameters based on laminate testes. The yarn material is a continuum damage mechanics (CDM) model utilizing either constituent damage properties [14] (micromechanical) or a homogenized macromechanical response [15] formulated for a unidirectional fiber reinforced polymer composite.

6 Boundary Conditions

Two related boundary condition methodologies are investigated for this analysis. The RVE boundary conditions described by Wang et al. [9] and those automatically calculated with a RVE capability implemented in our in-house finite element code Sierra. In general, the following describes the
boundary condition formulation for each method. First, the displacements on each parallel surface pair of the RVE rectangular prism as a function of Cartesian coordinates are given by

\[ u_i(x_1, x_2, x_3) = \bar{\varepsilon}_{ik} x_k + u_i^*(x_1, x_2, x_3) \]  \hspace{1cm} (9)

where \( \bar{\varepsilon}_{ik} \) are the average strains in the RVE. The second term on the right hand side \( u_i^* \) is a periodic function between RVEs ensuring continuity and is generally unknown. For linear elastic analysis, material constants can determined by simply applying displacement fields and periodicity which relies only on satisfying displacement differences on each pair of parallel faces. Thus, Wang et al. [9] shows that this equation reduces to

\[ u_i^{+} - u_i^{-} = \bar{\varepsilon}_{ik} (x_k^{+} - x_k^{-}) \]  \hspace{1cm} (10)

These boundary conditions are applied as periodic if \( \bar{\varepsilon}_{ik} = 0 \) or as displacements for the know (applied) quantities of \( \bar{\varepsilon}_{ik} \). Boundary conditions applied in a damaging medium are more complicated however. The above described methodology allows for multiaxial stress states, then solves for the stiffness tensor directly. However, with the exception of pure shear loading, damage parameter estimation requires uniaxial loading. Therefore, Equation 10, must be solved in order to ensure zero net traction in the unloaded directions. Since the in-house RVE method uses the strain rate (\( \dot{\varepsilon} \)), equation 10 is written as

\[ \dot{u}_i^{+} - \dot{u}_i^{-} = \dot{\bar{\varepsilon}}_{ik} (x_k^{+} - x_k^{-}) \]  \hspace{1cm} (11)

where \( \dot{\bar{\varepsilon}}_{ik} \) is the average strain rate over the RVE.

6.1 Elastic Verification

Two identical RVE meshes with elastic material parameters are implemented for each of the above described methodologies. First, six boundary conditions are applied as follows [9].

Six average strain tensors are applied to the faces of the RVE mesh. When \( \bar{\varepsilon}_{ik} = 0 \), the condition that \( u_i^{+} - u_i^{-} = 0 \) is ensured by periodic boundary conditions. The following provides the applied strain tensor and the output volume average stresses.

Six loading conditions are implemented to solve for the stiffness tensor. Shown here as columns of a 6X6 matrix

\[ \varepsilon = \begin{bmatrix} \varepsilon_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_{23} \end{bmatrix} \]  \hspace{1cm} (12)

The resultant stress tensors are written in matrix form as columns of a 6X6 matrix (\( \sigma \)). The elastic compliance of the system is calculated as

\[ S = \varepsilon \sigma^{-1} \]  \hspace{1cm} (13)

Symmetry is ensured and the elastic constants are solved from Hooke’s law for orthotropic materials.

The RVE capability uses a more direct route by applying conditions much the same way as experiments. The orthotropic homogenized elastic constants for a unidirectional composite with volume fraction 0.87 are calculated using the above formulations and shown to produce nearly identical results.

6.2 Damage Analysis

Damage initiation and propagation is assessed on the meso-scale RVEs using the homogenized finite element approach described in the previous section. For a given simple load case, such as cyclic load controlled, uniaxial, and various out-of-plane conditions, the boundary conditions are solved based
7 Results and Discussion

7.1 Elastic Properties

The macroscopic plain weave response is modeled and mechanically average for one set of statistical responses and compared to the plain-weave graphite-epoxy data presented in [11]. The easily measured in-plane yarn dimensions are sampled while the thicknesses and yarn shapes are determined by the balance of cross-sectional areas. This approach assumes uniform volume fraction in the yarn and an iso-phase layup.

A Latin Hypercube Sampling (LHS) of the characteristic parameters is used for model generation. Then a single layer structured mesh is used for macroscopic mechanical averaging, where each element is assigned one homogenized set of parameters from a single meso-scale representative volume. The warp elastic modulus ($E_{11}$) is given for one sampling of geometric parameters as 45.0 GPa, which matches well with the experimental responses. In general, a distribution of in-plane elastic responses is best obtained through experiments. However, the methodology presented here provides out-of-plane properties and insight into stress concentration for damage initiation and failure analysis. An example of transverse damage accumulation in a plain weave composite under pure in-plane shear is shown in Fig. 12.

Similarly, the homogenized elastic response of the 8 harness satin weave E-glass reduced unit cell predicts a range of warp modulus between 23.4 - 26.4 GPa for the manufacturer’s low and high fiber volume fractions respectively. This matches well with the experiments, where $E_{11} = 24.82$ GPa with a standard deviation of 0.56 GPa. The two sets of elastic parameters are shown in Table 1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Measured</th>
<th>Simulated</th>
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</thead>
<tbody>
<tr>
<td>$E_{11}$</td>
<td>24.82 ± 0.56</td>
<td>23.4 - 26.4</td>
</tr>
<tr>
<td>$E_{22}$</td>
<td>23.13 ± 0.39</td>
<td>21.1 - 25.0</td>
</tr>
<tr>
<td>$E_{33}$</td>
<td>N/A</td>
<td>8.78 - 10.4</td>
</tr>
<tr>
<td>$v_{12}$</td>
<td>0.13 ± 0.01</td>
<td>0.117 - 0.124</td>
</tr>
<tr>
<td>$v_{13}$</td>
<td>N/A</td>
<td>0.371 - 0.345</td>
</tr>
<tr>
<td>$v_{23}$</td>
<td>N/A</td>
<td>0.376 - 0.349</td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>3.71</td>
<td>3.40 - 4.47</td>
</tr>
<tr>
<td>$G_{13}$</td>
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</tr>
<tr>
<td>$G_{23}$</td>
<td>N/A</td>
<td>2.61 - 3.04</td>
</tr>
</tbody>
</table>

7.2 Damage/Plastic Properties from Shear

Responses not easily obtained using experimental methods are of primary interest. These include biaxial tension, compression, in and out-of-plane shear, residual stress distributions in curing, damage and plastic initiation and evolution, and off axis coupling effects. In the presence of limited data, simple experiments are used in addition to constituent properties to calibrate the meso-mechanical response. Figs 12 and 13 show the cyclic in-plane shear response of a plain weave RVE.
Plastic strains and damage evolution can be obtained from this homogenized response.

Fig. 12. Transverse damage distribution of a plain weave RVE under pure in-plane shear (shown without matrix)

For continuum damage evolution of the macroscopic homogenized material [1, 2]; coefficients describing Hill plasticity [16], crack closure and damage evolution are easily obtained using a series of RVE simulations.

Similar to the methodology presented in [1], the data is reduced to elastic damage and plastic strain evolution shown in Figs. 14 and 15 respectively. The calibrated coupled orthotropic elastic-plastic damage material model response is shown in Fig. 13. A statistical distribution of the parameters characterizing the variability of the responses can also be obtained.

Fig. 13. Cyclic shear response of a plain weave RVE

7.3 Tensile loading of 8HS GFRP

Transverse cracking of the weft yarns under warp direction tensile loading is marked by a knee in the stress-strain relationship (see section 3.4). Therefore, of interest is a statistical distribution of this stress state.

Micromechanical simulations are used to estimate the distribution of transverse failure strengths in the yarns based on geometrical variations. Matrix plasticity and failure are based on $J_2$ and maximum equivalent plastic strain criterion. The resulting random distribution of strengths are used to calibrate a continuum damage constitutive model [1, 2]. The transverse stress-strain curve is shown in Fig. 16.
Similar results are obtained when implementing the plain weave geometries given in [11]. Statistical distributions of geometries and constituent properties are easily included to obtain a range of meso-structural responses.

7.2 Interfacial debonding

Cohesive surface elements are used to simulate intralaminar debonding between the yarns and matrix. An in-plane shear loading simulation of a plain weave RVE, shown in Fig. 20, is provided as an example.

Fig. 20. Yarn interface debonding for a plain weave in shear (matrix is removed). The transverse shear stress is shown.

Buckling of the surface yarns under compression is difficult to predict. A reduced unit cell similar to those shown in [18] is generated in order to predict the local buckling of axial (warp) yarns on the surface of a beam loaded in four point bending. Figure 21 shows a carbon fiber laminate in four point bending with local buckling of surface yarns. Because our analysis focuses on glass fiber composites, which do not exhibit such behavior, the meso-mechanical simulations of this phenomenon remain under development. However, by using the capabilities developed in this study, a distribution of buckling loads can be determined from known geometric and material variability.
Fig. 21. Surface yarn interface debonding under axial compression (experiment).

7 Conclusions

An automated process for producing and pre- and post-processing geometrically accurate RVEs to obtain a distribution of constitutive responses has been presented using experimentally determined material and geometric measurements. Focus has been given on 2D woven composites, namely plain and harness weaves. Continuum yarn damage, inter-yarn debonding and an elastic-plastic matrix are combined with known materials and geometries in order to estimate the macroscopic response as characterized by a set of orthotropic material parameters. Elastic parameter estimation and validation along with a qualitative validation of damage/failure has been given. While much remains in terms of model and tool development and validation; the methodologies shown in this study provide a basis for material parameter estimation using a statistical RVE approach. The end user can estimate an array of parameters for design and material scoping exercises with minimal experimental effort.

References


