Virtual Specimens for Analyzing Strain Distributions in Textile Ceramic Composites

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Abstract

Methods are presented for calibrating the local elastic properties of tow-scale material domains in virtual specimens of textile composites. A model of the tow geometry is calibrated using 3D tomographic data via previously published methods. The local elasticity is defined to vary with the local tow orientation and fiber volume fraction within tows. The accuracy of the tow geometry is assessed by comparing the surface geometry of virtual specimens with an alternative data source, viz. topographical data obtained by digital image correlation (DIC). Calibration of the elastic constants is validated by comparing measured surface strain distributions with computed strain distributions. An approach is also presented for extending the model to the non-linear regime, by simulating the response of virtual specimens in which the bonds between abutting tows are broken and the resulting fracture surfaces are frictionless. The latter results yield a better match to the measured strain distributions.

Keywords: Fabrics/Textiles, Computational Modelling, Mechanical Properties, Surface Analysis

1. Introduction

Fabricating and testing textile ceramic composites is expensive and time consuming. To minimize cost and delay, computational models (virtual tests) are desired to inform and, to a substantial degree, replace experiments [1–3]. Since experiments show that cracking patterns in a textile composite are spatially correlated with the positions of individual tows [4–9], a virtual test must include heterogeneous material information at least down to the scale of tows, i.e., represent the tows as separate entities. Furthermore, the representation of tows should include stochastic variations in the local fiber orientation and volume fraction, the fiber tow shape and size, and the tow position; these

factors can influence local stresses and strains at the tow scale. In this work, we examine a material representation that includes these tow-scale characteristics. Furthermore, while homogenization is applied within each tow (i.e., discrete fibers are not represented), the material properties assigned within each tow may vary along the tow, because of variations in its orientation and cross-sectional geometry, and in the fiber packing density.

A method for generating stochastic virtual textile composites with tow-scale retention of material heterogeneity and implementing such virtual specimens in finite element (FE) models that predict local strains is presented in this article. The generating algorithm for the virtual specimens and a procedure for calibrating the local elastic properties of tows are validated by comparison with geometrical data and strain-field data acquired using digital image correlation (DIC).

The article continues a series that addresses the integration of experiments and theory to create a virtual test system for analyzing the behavior of textile ceramic composites under mechanical and thermal loads [3]. The series began with an article describing how x-ray micro-computed tomography (μ CT) images can be used to quantify the statistics of the geometry of fiber tows within a woven composite [10]. (Similar results have also been obtained for composites with 2D twill weaves [11].) The second article described how that statistical information is used to calibrate a one-dimensional (1D) virtual specimen generator, which uses a Markov Chain algorithm to describe local deviations of tows from average or “deterministic” trends throughout the composite material [12]. The tow loci are generated as 1D elements in three-dimensional (3D) space. A third article presented the exploitation of the Markov Chain algorithm in a 3D virtual textile specimen generator, with 3D representations of tows with stochastic shapes and positions [13]. Virtual specimens with 3D tow representations are the starting point for the present study. Other articles in the series reported the analysis and replication of stochastic tow positioning for specimens of sub-component size (ca. 0.1m x 0.1m) [14] and the calibration of the thermoelastic properties of the tows within a textile ceramic composite [15].

Over the years, approaches to representing the geometry of woven composites have progressed from assuming simple shapes for tows, such as rectangular segments arranged at approximately the correct weave angle [16–18], to more complex shapes that estimate tow cross-sections and weave paths from imaged specimens [19,20]. A key feature these methods lack is the ability to model stochastic variations in the weave architecture as determined from an experimental source. Other methods of geometrical modeling include simulations of the processing of textile

preforms, in which the compressive and shear deformation of individual tows is modeled [21,22]. Complications associated with this route include uncertainty about the loading conditions applied in weaving and in the subsequent handling of the fiber preform and the highly non-linear, generally unknown deformation response of bare fiber bundles to such loads [23–25].

In terms of mechanical modeling, many studies exist that show the accurate prediction of the spatially-averaged macroscopic properties of woven textiles using methods in which homogenization is applied at the laminate scale, i.e., individual tows are not represented [26,27]. Such approaches, however, may not be suitable for predicting strains at the local level. In woven fiber composites, experiments suggest that most failure mechanisms are associated with a length scale comparable to that of a single tow [4–7].

If failure mechanisms depend only on the average of the local strain field over a gauge length comparable to the tow width, predictions can be based on relatively coarse representations of tows. One such representation is provided by the Binary Model, which is constructed by embedding 1D tows, such as those generated by the stochastic Markov Chain algorithm [12], within 3D effective medium elements that fill out the external shape of a component. In the Binary Model, the 1D tow elements confer the axial stiffness of tows, while the effective elements confer the matrix-dominated contributions to global stiffness. When used in combination with gauge-averaging methods, the Binary Model can yield meaningful predictions of tow-scale variations in strains [7,28] and thence accurate predictions of failure in cases where ultimate failure follows in a quasi-brittle manner after the first local failure event occurs at the tow scale (e.g., rupture of a tow, kink failure of a tow in compression, or shear failure) [29,30]. However, the absence of 3D details of tow shapes renders the Binary Model incapable of tracking the full evolution of systems of interacting microcracks, such as trans-tow cracks, local delamination cracks between tows, and cracks in matrix domains. These complex microcracking systems govern failure in ceramic textile composites in high temperature and aggressive environments; their complete description is necessary for accurate life prediction [3].

The present article therefore addresses the construction of virtual specimens of textile composites based on 3D representations of tow geometry and the calibration of local elastic properties for individual tows within such virtual specimens. Calibration and most validation is restricted to the elastic regime. In the materials studied, which have non-smooth surfaces, elastic fields show strong, discontinuous variations that are correlated with the tow architecture. Simulations are extended into the early stages of the non-linear regime by considering the possibility

that debonding occurs between pairs of orthogonal tows. This phenomenon can arise at relatively low applied strains. Simulations of matrix microcracking, which contributes to substantial nonlinearity at higher strains, is beyond the scope of this work.

Construction of virtual specimens begins with the output from the generator based on 3D tow representations that was described in previous work [13], which we will refer to here as the *3D Virtual Textile Specimen Generator*, or *3D Virtual Specimen Generator* in short. The output from the *3D Virtual Specimen Generator* comprises a list of points and connecting facets that define tow surfaces. Surface profiles for each tow are extracted from the 3D mesh and compared to data for real test specimens obtained via DIC, providing a check on the geometry of the virtual specimen. To prepare the model for use in commercially available FE software, the tow surfaces are divided into 3D computational elements and each element is assigned calibrated elastic constants, with material symmetries dictated by the local direction of the tow axis. The predictive capabilities of virtual tests that are based on the calibrated virtual specimens are assessed by comparing strain fields measured by DIC with those computed by the FE model.

2. Acquisition of Experimental Data

2.1 Subject Material

The subject material is a three-layer angle interlock weave whose reinforcement consists of tows of T300-6k carbon fibers. The unit cell is comprised of four warp tows that undulate with staggered phases and twelve nominally straight weft tows. The fibers in the weave are first coated with very thin ($<0.1\mu\text{m}$) pyrolytic carbon by chemical vapor infiltration (CVI). CVI is then used to deposit a low volume fraction of SiC matrix. The process results in thin (ca $1\mu\text{m}$) SiC coatings on the individual fibers and thicker ($30\text{--}50\mu\text{m}$) SiC layers around the tows (**Figure 1**). The result is a highly porous but rigidified composite. Such materials have practical use in heat exchangers where flow is turbulent and some leakage is tolerable or transpiration is required [31]. Additional details of the weaving and processing procedures are presented elsewhere [10,12,13].

This material provides a severe test case for validating the virtual test, because its visible surface follows the complex topography of the textile reinforcement, and the strain fields developed under load exhibit high levels of heterogeneity, with sharp discontinuities where tows overlap one another.

2.2 Mechanical Test Setup

Dog-bone-shaped tensile specimens were laser-machined from a larger composite panel in both warp and weft orientations (*i.e.* the tensile loading direction is aligned with the longitudinal axis of the warp and weft tows respectively). The gauge sections were 25.4mm long and 12.5mm wide. The ends of the specimens were infiltrated with epoxy and allowed to cure under load to achieve flat surfaces. Fiberglass tabs, each 0.8 mm thick, were bonded to the specimen ends, to facilitate uniform load transfer from the grips to the specimen. In preparation for topography and displacement mapping, one surface of each specimen was first coated with a thin layer of white water-soluble paint. A speckle pattern of black paint was then applied with an airbrush. Two specimens were tested in each orientation at room temperature at a nominal strain rate of $3 \times 10^{-5} \text{ s}^{-1}$.

2.3 Topography and Displacement Mapping

Images for DIC were taken with a pair of digital cameras (Point Grey Research Grasshopper) with a resolution of 2448 pixels by 2048 pixels. Each camera used a Nikon ED AF Micro-Nikkor 70mm-180mm lens with the focal length set to 180 mm. The cameras were oriented with a 24° angle between them, a configuration that permits acquisition of 3D spatial information on the specimen surface. The offset distance was chosen as the minimum focal distance, which resulted in a final magnification of $7.7 \text{ } \mu\text{m/pixel}$. The width of a typical tow (approximately 1 mm) was therefore covered by approximately 100 pixels.

Each image sequence was subsequently correlated using VIC-3D software (Correlated Solutions). The correlation analysis is controlled by two parameters: the “subset” size and the “step” size. A “subset” of an image is a square patch over which correlations are computed to obtain a displacement of the patch relative to its position in the initial image of the sequence, which is attributed to the center point of the patch. For the purpose of the correlation calculation, the displacement is assumed to vary linearly with position over the patch area. A “step” refers to the distance by which the center of the patch is moved before the next correlation is computed and therefore establishes the separation of the mesh of points at which displacements are determined. For these tests, the subset and step sizes were 41 and 3 pixels, respectively. The choice of subset size was partly determined by the requirement that it be sufficiently large that correlations could be successfully computed across the entire specimen, which requires that a minimum number of image features fall within every subset. For smaller subsets, some surface regions could not be

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4 correlated in sequential images and hence the displacements in those regions could not be ascertained. The output
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6 dataset comprised measurements of relative surface height, $\Delta h(x,y)$, and in-plane displacements, $u(x, y)$ and $v(x, y)$,
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8 evaluated at an array of points, (x_i, y_i) , covering essentially the entire gauge area. Given that a pixel spans $7.7 \mu\text{m}$,
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10 displacements are determined at approximately 30 – 40 points across the width of a typical tow.

11 12 13 14 15 **3. Finite element model**

16 17 *3.1 Preliminaries*

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19 A previously published algorithm (the *3D Virtual Specimen Generator*) is used here to generate virtual specimens
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21 for which the statistics of local variations in tow geometry are matched to calibrating data for the subject materials
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23 [12,13]. In summary, data from micron-resolution x-ray computed tomography (μCT) were analyzed to yield
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25 statistical descriptors of the variance in position and cross-sectional geometry of all tows in a specimen that was
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27 nominally identical to the specimens studied here. A Monte Carlo reconstruction algorithm based on a Markov
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29 Chain formulation was then used to generate virtual specimens, i.e., instantiations of stochastic tow positions and
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31 shapes. A separate Markov Chain generator is used to generate each of five characteristics of each tow, namely two
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33 positional coordinates, which characterize random sideways deflections of the tow's center of mass, and the area,
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35 aspect ratio, and orientation of the tow's cross-section. Stochastic values of these characteristics are generated along
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37 the length of each tow, with statistics matched to the measured variance and correlation length (characteristic
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39 distance along a tow over which deviations remain significantly correlated). The deviations for different tows are
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41 treated as uncorrelated. The resulting stochastic geometrical tow model is then mapped onto a discrete mesh.
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43 Possible interpenetration and ordering errors that arise when the model of all stochastic tows is assembled into one
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45 model are removed by invoking topological ordering rules, which embody the topological definition (interlacing
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47 pattern) of the weave architecture.

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50 Given such a geometrical representation, it remains to prepare the virtual specimens for finite element simulations of
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52 composite behavior. This requires the generation of a finite element mesh and the calibration of local material
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54 properties. These tasks are the topic of this paper.

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56 Mesh generation is based on tetrahedral 3D elements. The tetrahedral elements allow the use of straightforward
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58 tessellation algorithms for describing irregular 3D shapes. They may also be best suited to future studies of the

development of multiple microcracks: e.g., one promising FE model formulation for crack simulations, the Augmented Finite Element Method (A-FEM) [32], is currently based on tetrahedral elements. However, the present work primarily addresses the elastic regime.

The calibration of local material properties must account for the local variations in tow orientation and fiber volume fraction within each tow. Micromechanical models (detailed in Appendix B) are used to compute such variations. Because the properties of ceramic matrices in the confines of a fiber composite are generally very different from those of monolithic specimens of nominally similar materials [28,29], a calibration test is also required to establish the Young's modulus of the "effective" matrix material. In the present composite, the effective matrix is a homogenized representation of the SiC coatings on the fibers and on the tows as well as the intra-tow porosity.

The generation of virtual specimens and their use in virtual tests in this paper consists of the following steps: use the *3D Virtual Specimen Generator* to make a geometrical model of a textile; convert the geometrical model to a mesh of tetrahedral elements; complete the virtual specimen definition by assigning local material properties to each tetrahedral element according to the local, correctly oriented tow properties; and validate the virtual specimen using virtual tests, i.e., simulations of the mechanical behavior of the composite, primarily in the elastic regime.

3.2 Mesh Generation and Model Formulation

The output from the *3D Virtual Specimen Generator* is a 3D description of the outer surfaces of all tows. To port this into a usable mesh for FE simulations, a procedure for generating solid 3D tows is required. Delaunay triangulation [33]¹ was employed to generate the mesh. Delaunay triangulations maximize the minimum internal angles of elements and thus tend to avoid high aspect ratios, which are undesirable in FE simulations. The software package *TetGen* (Version 1.4.3) [34] was used to generate the meshes. Controls exist within the software to allow for constraints governing maximum element volume and aspect ratio. This level of regulation permits various degrees of mesh refinement.

The input dataset is a list of surface facets and nodal locations for each fiber tow. This information is provided, without modification, by the *3D Virtual Specimen Generator*. The output is given as a list of tetrahedral element

¹ For an English language definition: http://en.wikipedia.org/wiki/Delaunay_triangulation

points and nodal locations for each tow. An example of an FE mesh is presented in **Figure 1(b)** for the experimental specimen shown in **Figure 1(a)**. This dataset can be ported directly to FE software.

The variation in tow strains observed in the real material is a function of: (i) experimental error; (ii) position in the specimen; (iii) local variation in material properties, (iv) local variation in contact conditions; and (v) stochastic variation in tow shape. For this study, two systematic virtual specimens were created, *i.e.*, without stochastic deviations. While the *3D Virtual Specimen Generator* is inherently capable of generating tow models with stochastic geometry, the study was focused on the variations in local strains that are caused by the presence of a textile architecture ((ii), (iii) and (iv) above), which are relatively large and can be predicted using a non-stochastic textile model. The study of stochastic virtual specimens will be the subject of future work.

The dimensions of each virtual specimen equal those of the gauge section in the experimental specimens (25.4mm x 12.5mm). One specimen had the warp tows oriented along the longest dimension and the second had the weft tows along the longest dimension. Tow-tow contact conditions were prescribed as either fully-bonded (tied) or fully-unbonded (frictionless). These two contact conditions represent the physical extremes (actual tow-tow contact behavior is likely to be complex, heterogeneous and non-linear). Simulations were performed of uniaxial tension tests along the main axis (x in the warp specimen, y in the weft specimen) using the *ABAQUS* FE software package (Version 6.12).

Additional details of the mesh, boundary and contact conditions are provided in Appendix A.

3.3 Assessment of FE mesh

Previous assessments of the *3D Virtual Specimen Generator* have been based on the ability of the algorithm to reproduce, in a large ensemble of instantiations, the statistics of μ CT data that had been used for calibration [12,13]. The surface profile data obtained from the present DIC analyses were used to further assess the fidelity of the geometric model against a separate data source.

Figure 2(a) and **(b)** show surface contour plots of both virtual and real test specimens. Qualitatively, the surfaces are a close match. **Figure 3** shows histograms of the corresponding relative surface height, $\Delta h(x, y)$. The histograms agree to a degree consistent with the size of the data set in key features of the distribution, *e.g.*, the location, size and

shape of the three peaks that correspond to each of the three tow genres. Line scans taken along the surface of real and virtual specimens (**Figure 4(a)**) show that the relative surface heights along a single tow path are accurately depicted by the virtual specimen, within about 10 μm . The slight differences may be attributed to the variations in the thickness of the SiC matrix around the tows, a feature not included in the virtual geometry. Overall the correlations between virtual and real surface topographies are deemed to be very good.

3.4 Local tow orientation

Due to symmetry, the tows are transversely isotropic. The plane of isotropy should lie perpendicular to the local fiber direction, which varies along the tow axis. The implied spatial variation in elastic properties is modeled by defining a local coordinate system aligned with the local fiber direction for each element.

Consider the case of warp tows, which are nominally aligned with the x -axis in the global coordinate system. Let (x_c, y_c, z_c) be the centroid of a computational element within a warp tow. The local coordinate system (x_L, y_L, z_L) for the element is defined as follows: First, the axis x_L is defined to pass through the pair of successive points (X_i, Y_i, Z_i) and $(X_{i+1}, Y_{i+1}, Z_{i+1})$ on the tow locus for which $X_i \leq x_c < X_{i+1}$. The tow loci points are provided by the *3D Virtual Specimen Generator*. Next, the axis y_L is defined to be orthogonal to x_L and co-planar with x_L and the global y -axis:

$$\mathbf{y}_L = \frac{\mathbf{e}_y - (\mathbf{e}_y \cdot \mathbf{x}_L) \mathbf{x}_L}{|\mathbf{e}_y - (\mathbf{e}_y \cdot \mathbf{x}_L) \mathbf{x}_L|} \quad (1)$$

where $\mathbf{e}_y = \{0, 1, 0\}$ is the base vector for the global y -axis. Finally, z_L is given by the following vector cross product:

$$\mathbf{z}_L = \mathbf{x}_L \times \mathbf{y}_L. \quad (2)$$

This axis system is generally rotated from the global coordinate system through modest angles. The same procedure is used to define a local coordinate system at each element within the weft tows, by interchanging x and y as well as x_L and y_L in Eqns. (1) and (2).

3.5 Spatial Variations in Tow Properties

Data from μCT images show that the tow cross-sectional area varies slightly along each tow. Since the number of fibers is constant, the local volume fraction of fibers and hence the elastic constants must therefore vary. The spatial

variations in elastic properties are predicted by the micromechanical models of the homogenized tow properties, detailed below.

4. Calibration Procedure

The elastic constants of the fiber tows are computed using established micromechanical models (detailed in Appendix B) in combination with the local fiber volume fraction and the known or experimentally determined properties of the constituent phases. The elastic constants of the T-300 carbon fibers are regarded as known *a priori*; the values used are those provided by the manufacturer (BP-Amoco chemicals) and summarized in **Table 1**. The fibers are themselves transversely isotropic and therefore five independent elastic constants are needed. In contrast, the elastic properties of the matrix material within the tows – a combination of pyrolytic carbon and SiC coatings on the fibers, a SiC jacket around the tows, and void space – cannot be readily specified *a priori*. Instead, they are obtained through a calibration procedure that makes use of the experimental stress-strain data for the composite. For this purpose, the matrix is treated as homogeneous and isotropic and therefore characterized by two elastic constants. The matrix Poisson's ratio (whose value has minimal effect on composite elasticity [26]) is assigned the value $\nu_m = 0.2$ [35]. The matrix Young's modulus, E_m , remains as the single scalar parameter that must be calibrated by the test data. Other elastic constants, such as the shear modulus, G_m , and the plane strain bulk modulus, k_m , that may appear in micromechanical models can be deduced from E_m and ν_m via [36]:

$$G_m = E_m/2(1 + \nu_m); \quad k_m = G_m/(1 - 2\nu_m). \quad (3)$$

Calibration is accomplished through a parametric study in which the Young's modulus of the effective matrix is varied over some range of values and, for each value, the elastic tensile stress-strain response is computed and compared to the small-strain linear-elastic portion of the corresponding measured stress-strain curve for the tests oriented parallel to the weft axis (up to $\varepsilon \approx 0.001$ in **Figure 5(b)**). Following this procedure yields $E_m \approx 100$ GPa. Validation is achieved through comparison of the virtual test and experimental results for specimens loaded parallel to the warp axis for $E_m = 100$ GPa (**Figure 5(a)**). A sensitivity study was conducted on the value of E_m and it was found that a large change in E_m ($\pm 50\%$) has a small effect on calculated strains ($< 10\%$).

The need to calibrate the matrix elasticity using the textile composite specimen contrasts with the case of polymer matrix textile composites. Processing methods for polymer matrices are so mature and effective that the matrix fills

all space in the composite and has a composition similar to that of neat specimens of the polymer. Since both the fiber and matrix elasticity can be treated as known *a priori*, micromechanical models lead to accurate *a priori* predictions of composite elasticity [6,26,37].

5. Assessment of Strain Distributions

5.1 Procedure for Strain Comparisons

With the single elastic constant that needs to be empirically calibrated having been determined from the global elastic response of the composite (**Figure 5**), the predictive capability of the FE model was further assessed by comparing local (tow-scale) strain variations obtained from the simulations and from experiments. To eliminate bias, the analyses of both experimental and simulation data sets were conducted using identical procedures, as described below.

The output from both the DIC experiments and FE simulations are sets of in-plane displacements $\{(u(x_i, y_i), v(x_i, y_i)), i = 1, \dots, N\}$ evaluated at an array of points $\{(x_i, y_i)\}$ covering the specimen surface over the entire gauge section. The position variables (x, y) constitute an imaginary flat surface lying parallel to the actual (non-flat) specimen surface. Because of the existence of near-vertical tow boundaries at the edges of individual tows that appear on the specimen surface, the displacement field may possess discontinuities when projected on (x, y) . Thus, strains computed from surface displacements can lack physical meaning near the tow boundaries. This feature is inherent to the present composite, which lacks the additional matrix material that would normally be added to produce a smooth outer surface (**Figure 1(d)**). The sparseness of the matrix also affects tow-tow contact within virtual specimens: only a portion of the overlapping tow areas are actually in contact (**Figure 6**).

Examples of displacement discontinuities are evident in the line scans of axial displacements from both the experimental and the FE data, presented in **Figure 4(b)**. In both datasets, the scans consist of several essentially linear sections, each lying within a single tow, separated by small displacement jumps at the tow boundaries.

To assure that physically meaningful quantities are obtained, strains are computed and averaged only over surface domains in which discontinuities are absent. The first step in the analysis is the subdivision of the specimen surface into domains associated with the visible segments of individual warp and weft tows, identification of the tow genus to which each domain belongs, and partitioning of the raw image data into individual tow domains (image

segmentation). As illustrated by the dashed boxes in **Figure 2(a)**, the domain attributed to a particular tow segment excludes a narrow region around the periphery in which the displacements, which are calculated by averaging over a gauge length (the subset size) centered on any point, would be affected by displacement discontinuities at tow boundaries or would sample the distinct displacement fields present on adjacent tows. If the width of the excluded zone is taken as one half of the subset size, all displacement sampling is confined to the single tow domain of interest.

Three types of tow domain are present on the specimen surface: warp, surface weft, and center weft [10]. The average strains within each domain are computed by fitting each displacement field, say $\{(u(x_i, y_i))\}$, to a bilinear function in x and y . The gradients of the fitting functions yield the strains $\{\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy}\}$; strains from equivalent domains are considered as a distribution representative of the domain type. The degree to which strains are uniform within each tow domain was assessed by calculating the coefficient of determination, R^2 , for the bilinear fit; it was found that the majority of strains calculated for tow domains corresponded to $R^2 > 0.8$. Thus strains were reasonably linear, but deviations from linearity do exist, as evident in **Figure 4(b)**, where experimental displacement data (red curves) for the higher applied strain value vary in a clearly non-linear manner within a single tow domain. Among predicted strain variations, one significant and interesting case of deviation from non-uniformity was found in simulations within a domain on a weft tow when loading was aligned with the warp direction, as detailed in Section 5.4. This case of non-uniformity notwithstanding, removing strains with $R^2 < 0.8$ arising within domains of any type did not significantly alter the overall degree of agreement between the computed and measured average strains within tow domains of any genus.

As described above, two tow-tow contact behavior models were simulated: (i) fully-bonded (tied) and (ii) fully-unbonded and frictionless. Further details pertaining to these contact models are presented in Appendix A.

5.2 General remarks on strains averaged across individual tow domains

The axial strains parallel to loading in the warp direction, ε_{xx} , for each type of tow domain (warp, surface weft and central weft) are summarized in **Figure 7** for two values of applied strain. The axial strains parallel to loading in the weft direction, ε_{yy} , are summarized in **Figure 8**. In both figures, the strain data, whether experimental or from simulations, refer to strains averaged over the dimension of the tow domain that is aligned with the load (therefore

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4 either the width or length of the tow domain) for each tow domain of any genus. The experimental results are
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6 presented in the form of box-and-whisker plots. In these plots, the bottom and top of the box represent the lower and
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8 upper quartiles of the data, respectively; the solid line within each box represents the mean value; and the ends of the
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10 whiskers represent minimum and maximum values. The predicted strains obtained via the FE model are represented
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12 as discrete points, one for each tow domain of the given tow genus that lies within the specimen.
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15 Because the simulations were executed for virtual specimens that contained no stochastic character, the distribution
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17 of the predicted strain values for a single tow genus in **Figure 7** and **Figure 8** (i.e., the column of points for one tow
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19 genus) reflect repeatable and consistent sources of variability: the strain in one domain of a tow genus varies
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21 because that domain has a unique relationship to adjacent tows, depending on its position within the unit cell of the
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23 textile architecture, and a different relationship to the boundary conditions in the specimen, which is not much larger
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25 than the unit cell.
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28 In contrast, variability in the experimental data is presumed to be the sum of such effects, the effects of stochastic
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30 material characteristics, and measurement noise. Stochastic material characteristics include the complex shapes of
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32 the boundaries (upper surfaces) of tows (**Figure 1(c)** and (d)). Such shape variance influences the distribution of
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34 stress within the tow and also compromises the accuracy of digital image correlation that is based on images from
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36 dual cameras that view along different lines of sight (Sect. 2.3). Distinguishing these two effects in experimental
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38 data, one effect being a real effect on stress distribution and the other a form of measurement noise, is difficult.
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41 A further source of variance in the averaged strains in tow domains, which is visible in simulations and presumed to
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43 be present in experiments, is variance in the contact areas between pairs of tows at different locations within the unit
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45 cell, which will influence stress distributions throughout the tows.
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48 Information about the finer details of the variations of tow cross-sectional shapes were not well quantified
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50 experimentally and were not replicated in the virtual specimens. Therefore, quantifying the degree to which each of
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52 the effects described above contributes to the variance in the experimental data for average strains in domains is not
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54 possible. However, we observe that the variance in experimental data is similar to but somewhat higher than the
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56 range of strains predicted in simulations (**Figure 7** and **Figure 8**), which is expected because not all sources of
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58 variance in the experimental data were represented in the simulations.
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One interesting case is that of weft tows that are aligned with the applied load, for which the *range* of predicted strain values is relatively narrow and several times lower than the variance in the experimental data (**Figure 8**). We discuss this case further below.

Overall, the cumulative effects of variations in local tow properties and the asymmetrical architecture on the distribution of strain values are reasonably well captured by the model.

Validation of the virtual specimens will rest primarily on comparing the mean values of strains for each tow genus. For loading parallel to the warp axis, at the lower applied strain ($\epsilon = 0.0005$, **Figure 7(a)**), the average measured values within each of the three domain types are similar to one another. Furthermore, their magnitude represents about 2/3 of the total macroscopic strain, the balance being accommodated by the displacement discontinuities at the tow boundaries. At a higher applied strain ($\epsilon = 0.002$, **Figure 7(b)**), the average measured value within each tow domain type becomes a smaller fraction ($\leq 1/2$) of the total strain. This trend is likely a result of reduced tow-tow contact (as a result of damage) and hence a progressive de-coupling between neighboring tows. Some portion of the reduced strain in the warp tows might also be the result of tow straightening² following damage at the tow-tow contacts.

Results for the tensile tests performed along the weft direction are summarized by the box-and-whisker plots in **Figure 8**, for applied strains of 0.0005 and 0.002. Here the measured axial strains in the center and surface wefts are similar to one another in magnitude and in range; and their averages are considerably higher than those measured within the warp tows (close to zero). This result on its own strongly suggests that the contacts between warp and weft tows are almost non-existent and thus no significant load can be transferred from the axial (weft) tows to the transverse (warp) tows.

5.3 Strains in tows aligned to loading

The strains in tows that are nominally aligned with the load axis are expected to follow the applied load approximately proportionately: these tows are gripped, either directly or indirectly, near the ends of the specimen and present continuous load pathways from one end of the specimen to the other. Therefore, comparison of the

² Recent computed tomography imaging of this material under tensile load aligned with the warp direction has revealed splitting cracks within the warp tows, which are confined to the regions where the warp tows are most inclined to the load axis (Bale, unpublished work, 2015). Such cracks are consistent with tow straightening.

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4 experiments and simulations for strains in the aligned tows should provide the most accurate assessment of the
5 calibration of the virtual specimen. Data from **Figure 7** and **Figure 8** are re-plotted as scatter plots in **Figure 9**, one
6 for aligned warp tows and one for aligned weft tows. In **Figure 9**, each tow domain in the specimen is represented
7 by one point.
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12 The strains that are predicted for any aligned tow genus are substantially different for the cases of bonded and
13 unbonded tow interfaces; and the two sets of predictions approximately bracket the experimental data (**Figure 7**
14 &**Figure 8**). Assessing the strains in aligned warp and aligned weft tows at the two values of applied strain ($\varepsilon =$
15 0.0005 and $\varepsilon = 0.002$), one finds that predictions for unbonded tow interfaces fall close to the experimental data in
16 all cases, and much closer to the data than predictions for bonded interfaces, with the exception of the case of
17 aligned warp tows at low applied strain ($\varepsilon = 0.0005$). This is also clear in the scatter plots of **Figure 9**. For the
18 exceptional case, the predictions for bonded and unbonded interfaces straddle the data. A possible explanation for
19 the exception may lie in friction effects between tows, which have not been modeled.
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30 We conclude that the interfaces between warp and weft tows in this composite are initially weak and fail early in
31 loading, or perhaps have already failed after processing. This condition is probably a peculiarity of this unusual
32 composite, which has so little matrix lying outside and between tows. A composite in which matrix was added to
33 fill out space to flat upper and lower specimen surfaces would probably not exhibit such behavior.
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39 Further, we conclude that the calibration of the elastic response of the virtual specimens is successful in that the
40 average strain in aligned tow domains predicted in simulations agrees with that measured experimentally, within the
41 variance in both. The agreement is achieved for loading in both warp and weft directions at applied strains up to
42 0.2% using a single unknown elastic constant, the effective matrix Young's modulus, which was calibrated using the
43 global response of the specimen.
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49 More complete understanding of the origin of tow interface effects requires analysis of the gradual progression of
50 debonding between pairs of tows at crossovers. Such debond cracks will possibly interact with other matrix cracks,
51 forming complex crack systems that influence the details of strain distributions [3,4,38]. A satisfactory analysis
52 requires formulations that deal realistically with such interacting crack systems in heterogeneous materials (e.g.,
53 [39–41]), as well as the representation of stochastic variations in tow position and geometry, which tend to influence
54 the onset of cracking more strongly than they influence elasticity in uncracked materials [3].
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5.4 Strains in tows not aligned to loading

Tows that are nominally orthogonal to the load axis are not directly coupled to the applied load, but are loaded indirectly via their interfaces with the nominally aligned tows. Therefore, the strains in orthogonal tows are likely to be strongly influenced by the interfacial coupling between warp and weft tows, which, as inferred above, is weak and uncertain.

A striking illustration of the complexity of possible tow-coupling effects is presented by the strains calculated in weft tow domains in simulations where loading is aligned with warp tows: the strains in the weft domains are predicted to be negative in the case of unbonded tow interfaces (**Figure 7**). This phenomenon is most pronounced for the center weft tow genus and at the lower strain level ($\varepsilon = 0.0005$), but is present for some surface weft domains, and at the higher strain level ($\varepsilon = 0.002$). Examination of the strain distribution within the surface weft domains (e.g. **Figure 10(a)**) indicates the presence of a diagonal band of compressive strain across the domain. Inspection of the contact areas (**Figure 10(b)** and (c)) associated with orthogonal warp tows surrounding the center weft tow shows an approximately anticlastic loading condition (bending around two orthogonal axes in opposite directions) [42,43], which results in compression of the surface layer of the center weft tow domain. The band of surface-layer compression is the strain reported in **Figure 7**, averaged over the domain.

The absence of compressive strain values in the experimental data implies that different weft-warp contact conditions exist in the real specimen. In the virtual specimen, contact is restricted to a pattern of relatively small areas (**Figure 10(b)**), but, in the virtual specimens, no matrix at all was added to fill out inter-tow interstices. In the real material, a small quantity of matrix was added to the surfaces of tows and even a small quantity can strongly affect the contact areas between pairs of warp and weft tows. If the contact area covers the width of the tows more or less completely, the condition of anticlastic loading that arose in the simulations will not exist.

The analysis of strains in warp tow domains for loading in the weft direction is more straightforward: the predicted strains for the case of unbonded interfaces match the experimental observations. First, the contact area between a warp tow and weft tows within a domain of the warp tow that is visible and available for measurement tends to consist of a single larger patch (**Figure 6(b)**). Therefore the rather exotic multi-point loading effect described in **Figure 10** for center weft tows does not arise. Second, the nominally straight weft tows have a relatively small influence on the warp tows through direct contact. This is in contrast with the warp loading case where straightening

of the warp tows transfers a contact pressure to weft tows. Thus the predictions for the unbonded case, which were inferred in Sect. 5.3 to be the correct case, ought to match experiment for warp tow domains under loading in the weft direction; and they do (**Figure 8**, warp tows).

For similar reasons, predicted strains in surface weft tows for loading in the warp direction are not far from the measured strains (**Figure 7**, surface weft tows); the contact area with surrounding warp tows is much larger than for center weft tows (**Figure 6**), minimizing bending effects, although these effects still yield predictions of negative surface strains in one or two domains of the surface weft genus.

Full understanding of this complex relationship requires a detailed analysis of strain distributions due to varying levels of tow-tow contact, including a systematic and stochastic representation of contact areas and simulations of damage progression at the tow-tow interface.

6. Conclusions

The *3D Virtual Textile Specimen Generator* introduced in [13] is capable of creating replicas of stochastic 3D specimens of a woven textile composite using an input dataset provided by experiments. The generator produces unique instantiations, or virtual specimens, that each match the experimentally determined statistics of the stochastic reinforcement geometry (data from [10]). It can readily generate large ensembles of such virtual specimens by employing a robust algorithm that is also easy to use.

Characteristics of the surface of the virtual specimens, including the relative surface height and the displacements and strains induced by load, are all analyzed in exactly the same manner as experimental data. This allows unambiguous comparison of results and yields a robust method of validation of the model, which was very successful in the present study.

Local strains within individual tows that are nominally aligned with the load axis are predicted well in the elastic regime using only a simple calibration of an effective Young's modulus for the matrix within fiber tows based on the global response of a composite test specimen (**Figure 5**).

The onset of material non-linearity due to debonding of the tow-tow interface was simulated using a frictionless contact condition, which demonstrated the importance of load transfer at tow crossovers to local strain variations.

In particular, we infer that in the real specimens analyzed, warp and weft tows are debonded from one another either at very low applied loads or after processing.

In this unusual composite with sparse inter-tow matrix, non-uniform contact between warp and weft tows in simulations can generate curious strain variations in tows that are orthogonal to the load axis, including locally negative strains in the direction of loading. The extreme condition of zero inter-tow matrix required for this effect to occur was not present in the real specimens analyzed (which had a modest amount of inter-tow matrix, rather than zero inter-tow matrix) and therefore negative strains were not measured experimentally. Nevertheless, the analysis points out how complex the local strain state can be in sparse-matrix composites. Such composites have significant potential applications in heat exchangers, such as combustor liners, where leakage and non-smooth surfaces are acceptable (even preferable).

Simulations of multi-crack damage progression are currently being undertaken, within which the ability of the virtual specimen generator to replicate material variability will be used to study the effect of such variability on failure.

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Appendix A. Meshes, boundaries and contacts

The FE meshes, after successful mesh convergence, comprise 499,378 nodes and 2,423,600 tetrahedral elements in the warp orientation, and 149,000 nodes and 558,412 tetrahedral elements in the weft orientation (**Figure A1**). The boundary conditions for loading parallel to the warp axis are as follows:

- (i) All nodes at $x = 0$ mm are constrained to have $u = 0$ mm.

- (ii) To simulate the grips present in the experiment, all nodes on the y - z plane at $x = 0$ mm and $x = 25.4$ mm are constrained to have $v = w = 0$ mm.
- (iii) An incrementally increasing displacement is applied on all nodes at $x = 25.4$ mm.

Analogous boundary conditions are used for the specimen loaded parallel to the weft axis. They can be expressed by exchanging x with y and u with v in the preceding description.

Tow-tow contacts were treated in one of two ways:

- (i) *Fully-bonded (tied)*: Nodes on the tow surface that are in direct contact with another tow are constrained to have the same displacement as that tow at that location. This is accomplished through the mesh tie constraint (*TIE) within *ABAQUS* where tow surfaces are paired in a master-slave configuration. (A slave tow in contact with a master tow is prescribed the same displacement as the master tow at that location).
- (ii) *Fully-unbonded and frictionless*: This behavior is prescribed through a surface contact interaction where both normal and tangential properties must be stipulated. Normal behavior is set to *hard* contact. This pressure overclosure prevents interpenetration of contacting tows and does not allow the transfer of tensile stress across the interface. With this contact condition, surface nodes are permitted to separate after contact. Additionally, the friction coefficient for tangential motion is set to zero.

Appendix B. Micromechanical models for elastic tow properties

Due to their symmetrical nature, fiber tows are inherently transversely isotropic with stiffness dominant along the longitudinal fiber axis. Therefore, the elasticity of the tow is characterized by five elastic constants. These are E_x , $E_y = E_z$, $G_{xy} = G_{xz}$, $\nu_{xy} = \nu_{xz}$ and ν_{yz} . Several micro-mechanics based approaches to calculate these elastic properties exist within the literature. Additionally, FE simulations of individual fiber tows can also yield the requisite properties [44]. For this study, FE simulations are unsuitable since the matrix properties are not known *a priori*. It would therefore require an inordinate amount of simulations and processing time to calibrate the desired properties. A more practical method of calculation is the use of one of the many available analytical models for describing elastic properties of fiber composites. An examination of several of these approaches is discussed in [26]. Hashin's [36] composite cylinder assemblage (CCA) model was selected for use since it explicitly considers anisotropic fibers.

Closed-form predictions for the parameters E_x , $G_{xy} = G_{xz}$, $\nu_{xy} = \nu_{xz}$ and k are attainable for transversely isotropic fibers in an isotropic matrix and are given by:

$$E_x = E_{f\parallel}f + E_m(1-f) + \frac{4(\nu_{f\parallel} - \nu_m)^2 f(1-f)}{\frac{(1-f)}{k_{f\perp}} + \frac{f}{k_m} + \frac{1}{G_m}} \quad (B1)$$

$$\nu_{xy} = \nu_{f\parallel}f + \nu_m(1-f) + \frac{(\nu_{f\parallel} - \nu_m)\left(\frac{1}{k_m} + \frac{1}{k_{f\perp}}\right)f(1-f)}{\frac{(1-f)}{k_{f\perp}} + \frac{f}{k_m} + \frac{1}{G_m}} \quad (B2)$$

$$G_{xy} = G_m + \frac{f}{\frac{1}{G_{f\parallel} - G_m} + \frac{1-f}{2G_m}} \quad (B3)$$

$$k = k_m + \frac{f}{\frac{1}{k_{f\perp} - k_m} + \frac{1-f}{k_m + G_m}} \quad (B4)$$

The subscripts $\parallel$ and $\perp$ refer to axial and transverse properties of the fibers and f is the fiber volume fraction.

Closed-form solutions for the remaining parameters $E_y = E_z$ and ν_{yz} are not attainable and are instead given by the mean of upper and lower bounds, which for the subject materials are reasonably close. Bounds for transverse Young's modulus, E_y , and Poisson's ratio, ν_{yz} , are given by

$$E_{y(\pm)} = \frac{4kG_{yz(\pm)}}{k + mG_{yz(\pm)}} \quad (B5)$$

$$\nu_{yz(\pm)} = \frac{k - mG_{yz(\mp)}}{k + mG_{yz(\mp)}} \quad (B6)$$

where $m = 1 + \frac{4k\nu_{xy}}{E_x}$ and for $G_{f\perp} < G_m$ and $k_f < k_m$ (as is the case for the material system of present interest), the upper and lower bounds for the transverse shear modulus, $G_{yz(\pm)}$ are given by

$$G_{yz(-)} = G_m \left[1 + \frac{(1+\beta_1)f}{\rho-f \left(1 + \frac{3\beta_1^2(1-f)^2}{\alpha f^3 - \beta_1} \right)} \right] \quad (B7)$$

$$G_{yz(+)} = G_m + \frac{f}{\frac{1}{G_{f\pm} - G_m} + \frac{k_m + 2G_m}{2G_m(k_m + G_m)}(1-f)} \quad (B8)$$

where $\pm$ represents the upper or lower bound and $\alpha = \frac{\beta_1 - \gamma\beta_2}{1 + \gamma\beta_2}$; $\rho = \frac{\gamma + \beta_1}{\gamma - 1}$; $\beta_1 = \frac{k_m}{k_m + 2G_m}$; $\beta_2 = \frac{k_f}{k_f + 2G_{f\pm}}$; $\gamma = \frac{G_{f\pm}}{G_m}$.

For this study, the constituent fiber properties (**Table 1**) are entered into equations B1-B8 along with a range of effective matrix properties. These properties are then input into FE simulations and the macroscopic composite Young's modulus is calculated and compared with experimental data (**Figure 5**). The input value of fiber volume fraction is inversely proportional to the cross-sectional area along each individual tow. This results in variable elastic constants along each of the fiber tows, which are input into the model.

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Figure 1. (a) 3D micro-CT image, (b) example 3D finite element mesh of experimental specimen (fine meshes and larger specimens used in simulations of test are shown in appendix A), (c) optical micrograph of a polished cross-section in the x - z plane and (d) magnified region showing disconnected tow boundaries that lead to displacement discontinuities.

Figure 2. Surface contour plots of (a) virtual and (b) real specimens. Rectangles in (a) denote the three types of tow domain. Dashed line shows location of line scan in **Figure 4**.

Figure 3. Histograms of relative surface height of virtual and real specimens. The peaks, from left to right, correspond to center weft, surface weft and warp tows.

Figure 4. Line scans of (a) relative surface height and (b) axial displacement (along dashed lines in **Figure 2**) in virtual and real specimens loaded along the warp axis (x). The data have been normalized so that the origins of each axis represent the median values.

Figure 5. Calibration of matrix Young's modulus, E_m , through comparisons of computed and measured stress-strain curves for loadings parallel to both the (a) warp and (b) weft axes. Datasets of the same colour represent individual tensile specimens. The simulations assume perfectly-bonded tow-tow contacts. Also shown are predictions of the stress-strain curves assuming unbonded tow-tow interfaces for $E_m = 100$ GPa.

Figure 6. Example of tow-tow contact for a virtual specimen in the (a) xz and (b) xy planes. Contact is denoted by solid red facets.

Figure 7. Box-and-whisker plots showing experimental distributions of tow strains at macroscopic applied strains of (a) 0.0005 and (b) 0.002, for loading *parallel to the warp* tow axis (x). The simulations include limiting cases (in terms of contact) in which tows are either perfectly-bonded or fully unbonded and frictionless. Predicted strains are shown as discrete points for each individual tow domain.

Figure 8. Box-and-whisker plots showing experimental distributions of tow strains at macroscopic applied strains of (a) 0.0005 and (b) 0.002, for loading *parallel to the weft* tow axis (x). The simulations include limiting cases (in terms of contact) in which the tows are either perfectly-bonded or fully unbonded and frictionless. Predicted strains are shown as discrete points for each individual tow domain.

Figure 9. Comparison of strains in tows aligned to loading for equivalent domains in the virtual and experimental specimens. (a) Strains in aligned warp tows (black = 0.0005; red = 0.002), and (b) strains in aligned weft tows (black = surface wefts at 0.0005; red = centre wefts at 0.0005; green = surface wefts at 0.002; blue = centre wefts at 0.002).

Figure 10. (a) Contour plot of strains parallel to loading (x); (b) schematic highlighting negative strain region in center weft tow domain and location of contact between the weft and warp tows. Red points represent overlying warp tows and blue points denote underlying warp tows; (c) schematic showing contact forces on weft due to crossing warp tows.

Figure A1. Converged virtual specimen mesh for loading (a) parallel to warp (x) axis and (b) parallel to weft (y) axis.

Table 1. Elastic Properties of T300-6k Carbon Fibers.

Young's Modulus ¹		Shear Modulus ¹		Bulk Modulus ²	Poisson's ratio		Volume fraction ⁴
$E_{f\parallel}$	$E_{f\perp}$	$G_{f\parallel}$	$G_{f\perp}$	$k_{f\perp}$	ν_f^1	$\nu_{f\perp}^3$	f
230GPa	14.5GPa	22.75GPa	4.8GPa	15GPa	0.27	0.51	0.61

¹BP-Amoco chemicals

$$^2 E_{f\perp} = \frac{4k_{f\perp}G_{f\perp}}{k_{f\perp} + mG_{f\perp}}, \quad m = 1 + \frac{4k_{f\perp}\nu_{f\parallel}^2}{E_{f\parallel}}$$

$$^3 \nu_{f\perp} = (E_{f\perp}/2G_{f\perp}) - 1$$

⁴Average tow fiber volume fraction calculated from μ CT images.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9

(a)

(b)

Figure 10

Figure A1

(a)

(b)