Effect of resin-rich zones on the failure response of carbon fiber reinforced polymers

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\textbf{A B S T R A C T}

We study the impact of size and spatial arrangement of resin-rich zones on the failure response of a carbon fiber reinforced polymer (CFRP) subject to loadings applied in the direction transverse to the fibers. An automated computational framework is utilized for the finite element (FE) modeling and simulation of damage process. The proposed approach relies on a packing-optimization algorithm to virtually reconstruct three large Statistical Volume Elements (SVEs) of CFRP with varying size and distribution of resin-rich zones, as observed in the imaging data. A parallel, non-iterative mesh generation algorithm is employed to create high fidelity FE models. The failure analyses are carried out considering the ductile damage response of the polymer matrix, as well as cohesive debonding and contact along fiber-matrix interfaces. The study shows that although the presence of resin-reach zones does not highly affect the failure response under transverse tensile and shear loads, it has a notable impact on the strength and toughness under transverse compression. Further, we show that using different boundary conditions and changing the compressive load direction (i.e., parallel versus perpendicular to the lamina) have a notable impact on the failure response of SVE.

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\section{1. Introduction}

Fiber reinforced composite (FRCs) have a wide range of applications in industries such as the aerospace and automotive. In these composites, embedded fibers (carbon, glass, ceramic, etc.) significantly enhance the mechanical properties of the matrix phase (polymer, ceramic, metal, etc.) without a notable increase in density. However, most FRCs have a certain level of microstructural uncertainty in the form of variations in the spatial arrangement and shape/size distribution of fibers, which could lead to uncertainty in the mechanical behavior. In particular, this feature has a notable impact on the failure response of FRCs, as the damage (e.g., micro-cracks in the matrix and fiber-matrix debonding) initiates at the sites of stress concentrations governed by the shape and size of fibers, as well as their relative distances (Kailasam et al., 1997; Byström, 2003). While numerical techniques such as the finite element method (FEM) are increasingly utilized to simulate the micromechanical behavior of FRCs, statistically capturing the impact of microstructural uncertainties on their failure response remains a major challenge. Most of previous modeling efforts rely on the idealization of the composite microstructure, without realistically incorporating geometrical features and distribution of fibers (Okabe et al., 2011; Romanowicz, 2012; Greco et al., 2013). Even among studies that have properly addressed this issue (González and Llorca, 2007; Totry et al., 2008b; 2010; Vaughan and McCarthy, 2011; Melro et al., 2013), the vast majority are limited to analyzing one single or at best a handful of microstructural models. Also, in most cases the analyzed models cannot be considered as representative volume element (RVE) of the FRC. Thus, the resulting data are statistically inadequate in terms of both the size of model and number of simulations to quantify the impact of uncertainties.

In terms of the modeling approach, multiscale numerical methods (Li and Chou, 2006; Llorca et al., 2011) are commonly used to predict the failure response of FRCs. An RVE is defined as the smallest volume element that is large enough to capture the material response in an averaged sense while statistically preserving the geometrical complexity of the heterogeneous media (Ostoja-Starzewski, 2002). In the context of multiscale FEM, the FE$^2$ method (Feyel, 1999; 2003) is one of the most popular techniques. In this concurrent multiscale method, the stress state at
each quadrature point of elements discretizing the macroscopic model is evaluated by simulating the failure response of a corresponding RVE subject to a macroscopic strain. The method is formulated based on a coupled information transfer between the macro and micro scales, while simultaneously solving the corresponding boundary value problem (BVP) at both scales. The FE2 technique has been implemented to simulate the damage response of a variety of heterogeneous composites, including carbon fiber reinforced polymers (CFRPs) (Raghavan and Ghosh, 2005; Ghosh, 2008; Ghosh et al., 2009; Greco et al., 2014).

Given the high computational cost of concurrent multiscale methods, the computational homogenization (CH) theorem, also referred to as the hierarchical homogenization, is more frequently employed to derive the macroscopic stress-strain response of FRCs (Totry et al., 2008b; Melro et al., 2013; Soni et al., 2014; Ahmadian et al., 2017). Compared to concurrent techniques, where both the micro and macro scales must be solved simultaneously, in CH the link between scales is established by passing information from the micro to macro scale only. Thus, although at the price of a lower fidelity for the macroscopic simulation, using a homogenization technique would significantly reduce the computational cost.

In CH, the stress-strain response is averaged over a finite solution domain, which is either a unit cell of a (presumably) periodic microstructure or an RVE (Kanit et al., 2003; Geers et al., 2010; Matouš et al., 2017). It is generally understood that CH methods provide an accurate prediction of macroscopic properties if the principle of the separation of scales holds true. A corollary of this principle in first-order CH methods (assuming constant macroscopic stress/strain at the microscale) is that the size of RVE must be considerably smaller than characteristic length scales of the macroscopic domain. RVE-based homogenization is well studied by several researchers to obtain effective properties of a variety of heterogeneous materials, see for example (Trias et al., 2006; Canal et al., 2012; Harper et al., 2012; Mirkhalaf et al., 2016; Mosby and Matouš, 2016; Herráez et al., 2018).

For most practical applications, the size of the microscopic domain analyzed in the CH method is restricted by the computational power and/or numerical challenges such as convergence. Therefore, dimensions of the analyzed model could be smaller than the minimum size needed to be considered as RVE. To overcome this limitation and following the terminology presented in Ostoja-Starzewski (2006), statistical volume elements (SVEs) are proposed and widely used in several CH-based numerical studies (Segurado and LLorca, 2006; Yin et al., 2008; Saneei and Fertig III, 2015; Abedi et al., 2017a; 2017b). While smaller than a conventional RVE, the SVE size must be large enough so that an ensemble of them is equivalent to an RVE. The impact of the SVE size and its boundary conditions on resulting homogenized properties are studied in Kanit et al. (2003) and Bahmani et al. (2019). Note that using SVEs instead of RVEs to estimate homogenized material properties provides random continuum fields, which in turn also allows analyzing the impact of microstructural uncertainties on the failure responses.

In either the concurrent multiscale analysis (e.g., the FE2 method) or the CH approach, the fidelity of simulation is highly dependent on realistically modeling the microstructural features of the FRC. One could build the model directly based on imaging data such as micro-computed tomography (micro-CT) or scanning electron microscopy (SEM) images (Buffiere et al., 1997; Kastner et al., 2011; Martin-Herrero and Germain, 2007), which theoretically yields the most realistic representation of the microstructure. In practice, however, preparation of such imaging data is expensive and often they lack the desired resolution/contrast to properly distinguish all material interfaces in complex microstructures (e.g., due to close proximity of fibers). Alternatively, virtual reconstruction algorithms relying on statistical microstructural descriptors (Torquato, 2002; Xu et al., 2014; 2015) or correlation function-based techniques (Kumar et al., 2008; Liu and Shapiro, 2015) can be implemented to address this issue. The implementation of these algorithms often involves the virtual packing of fibers in the domain (Hinrichsen et al., 1986; Ghosh et al., 1997; Wang et al., 2016), together with an optimization phase to replicate target statistical microstructural descriptors (Matouš et al., 2000; Lee et al., 2009) such as volume fraction and spatial arrangement of fibers. This process becomes computationally demanding in the presence of microstructural uncertainties such as resin-rich zones, as in addition to the increased size of RVE a larger number of statistical descriptors must be considered during reconstruction (Yin et al., 2008).

Despite the challenges enumerated above, it is still feasible to virtually create a sufficiently large, realistic microstructural model (RVE) that takes into account the impact of uncertainties using either a direct image-based reconstruction approach or a reconstruction algorithm. However, for many composites, including the CFRP studied in this manuscript, the exceedingly large size of resulting RVE could lead to two detrimental challenges: (i) simulating the failure response of the corresponding FE model would be highly computationally demanding, and even worse, the numerical convergence might be impossible; (ii) characteristic length scales of RVE are no longer significantly smaller than those of the macroscopic domain, which violates the principle of the separation of scales mentioned previously (Michel et al., 1999; Miehe and Koch, 2002). Either of these challenges does not allow the use of an RVE and instead necessitates implementing an SVE-based homogenization approach to statistically characterize random fields such as the stiffness and strength by performing multiple simulations.

The main objective of this work is to quantify the impact of size and spatial arrangement of resin-rich zones on the failure response of a CFRP ply subject to loadings applied in the transverse fibers direction. The uncertainty associated with the shape and size of these regions leads to variation in the volume fraction and spatial arrangement of surrounding fibers, which in turn affects the failure response. This study relies on the high fidelity FE simulation of the damage process (fiber-matrix debonding Hobbiebrunken et al., 2006; Yang et al., 2012 and continuum ductile damage in the matrix Totry et al., 2008a; Davila et al., 2005) in three virtually reconstructed large SVEs of the composite. These SVEs are composed of hundreds of fibers and a high length-to-width ratio, as CFRP lamina has a small thickness that restricts the SVE width. Failure analyses are then carried out considering tensile, compressive, and shear loadings applied in the transverse fibers direction. For the case of transverse tension and compression, we also study the impact of boundary conditions and loading direction (perpendicular to either width or length of SVE) on the strength and toughness of CFRP. It must be noted that the damage initiation in CFRPs is also affected by high stress concentrations near defects such as pre-existing pores (Chevalier et al., 2016; 2019b). However, based on the imaging data prepared for the CFRP system studied in this work, we assume the microstructure is defect-free and only study the impact of resin-rich zones on the failure response.

The remainder of this manuscript is structured as follows: Governing equations for the computational homogenization, as well as the continuum and cohesive-contact damage models used for failure analysis are presented in Section 2. Microstructural uncertainties in the CFRP system studied in this manuscript and challenges they impose on defining an RVE of the composite material are discussed in Section 3. We provide a detailed explanation of the automated modeling process in Section 4, involving the virtual microstructure reconstruction algorithm (Yang et al., 2018) and non-iterative parallel mesh generation (Soghrati et al., 2017; Nagarajan and Soghrati, 2018). Section 5 is dedicated to investigating the effect of resin-rich zones on the failure response subject to
to transverse loads, as well as the impact of the loading direction and boundary conditions on simulation results. Final concluding remarks are presented in Section 6.

2. Problem formulation

2.1. Computational homogenization

Assume $\Omega$ refers to the macroscopic domain of a cross-ply CFRP panel characterized in the macroscopic coordinate system $\mathbf{x}_m$. The SVE domain $\Theta$ corresponding to one of the CFRP lamina is defined in the microscopic coordinate system $\mathbf{x}_M$. The SVE domain $\omega$ is characterized by the characteristic lengths $l_m$ and $l_n$ associated with the macroscopic (CFRP panel) and microscopic (SVE) domains, respectively, the requirement to ensure that the scaled lengths are of marginal importance in a homogenization-based analysis is

$$\frac{l_m}{l_n} \ll 1,$$

where $\xi$ is the asymptotic scaling parameter. By satisfying (1), without a significant impact on accuracy, we approximate the displacement field $\mathbf{u}(\mathbf{x}_M, \mathbf{x}_m)$ in the CFRP subject to external loads using a first-order asymptotic expansion as

$$\mathbf{u}(\mathbf{x}_M, \mathbf{x}_m) = \mathbf{u}_M(\mathbf{x}_M) + \xi \mathbf{u}_m(\mathbf{x}_M, \mathbf{x}_m),$$

where $\mathbf{u}_M(\mathbf{x}_M)$ and $\mathbf{u}_m(\mathbf{x}_M, \mathbf{x}_m)$ are macroscopic and microscopic displacement fields, respectively. Note that for brevity, in this section we skip the well-known linear elasticity governing equations linking displacement vectors to external loads at each scale (refer to Matouš et al. (2008) for more details).

By decomposing the strain tensor similarly to the displacement vector, the Hill-Mandel micro-homogeneity principle (Hill 1985) can be employed to equate the macroscopic energy density $\Phi_M$ at a given point to the average macroscopic energy density $\Phi_m$ at its corresponding SVE as

$$\inf_{\Phi_m} \Phi_M(\mathbf{e}_M) = \inf_{\phi_M} \int_{\Theta} \Phi_m(\mathbf{e}_M + \mathbf{e}_m) \, d\Theta,$$

such that

$$\Phi_M = \frac{1}{2} \mathbf{e}_M : \sigma_M, \quad \Phi_m = \frac{1}{2} (\mathbf{e}_M + \mathbf{e}_m) : \sigma_m,$$

where $\mathbf{e}_M (\sigma_M)$ and $\mathbf{e}_m (\sigma_m)$ are macroscopic and microscopic strain (stress) tensors, respectively ("inf" stands for infinity).

The macroscopic strain tensor at each point in the CFRP panel can then be evaluated as an average of the microscopic strain field within its corresponding SVE, which can be written as

$$\mathbf{e}_M(\mathbf{x}_m) = \frac{1}{|\Theta|} \int_{\Theta} \mathbf{e}_m(\mathbf{x}_m) \, d\Theta.$$

The equation above, which is also known as the strain averaging theorem, would hold if appropriate boundary conditions (BCs) such as prescribed displacement, applied traction, or periodic BC is applied along SVE boundaries. While the latter is shown to be most effective in minimizing unrealistic stress concentrations along domain boundaries (Inglis et al., 2008), due to lack of geometrical symmetry in the SVEs studied in this work, we have used a combination of prescribed displacement and traction BC to simulate each type of loading. For example, in order to apply compression in the $y$ direction (vertical), the bottom edge is constrained against displacement in this direction, a prescribed downward displacement is applied along the top edge, and the two sides edges are considered traction free. We can then approximate $\sigma_M$ at each point of the macroscopic domain as

$$\sigma_M(\mathbf{x}_m) = \frac{1}{|\Theta|} \int_{\Theta} \sigma_m(\mathbf{x}_m) \, d\Theta.$$

In a homogenization-based micromechanical analysis, (5) and (6) are used to evaluate the macroscopic stress-strain response of a CFRP based on microscopic stress and strain fields approximated in an SVE. The CFRP studied in this work demonstrates a nonlinear macroscopic stress-strain response subject to loadings in the transverse fibers direction, which is attributed to the ductile damage evolution in the epoxy matrix (Section 2.2) and debonding along fiber-matrix interfaces (Section 2.3).

2.2. Ductile damage in the matrix

While cured epoxy shows a semi-brittle failure response under tension, it undergoes significant plastic deformation before the initiation and evolution of damage subject to compressive and shear loads (Hooputra et al., 2004; Sadowski et al., 2014). Thus, the failure response of each lamina of CFRP also exhibits a ductile behavior under these loading conditions. In order to simulate this behavior, we implement a phenomenological continuum ductile damage model that takes into account both the elasto-plastic deformation response and the initiation/propagation of cracks based on the concept of void nucleation, growth, and coalescence. In this model, the yield surface is defined as

$$f(\sigma) = q - \sigma_p(\varepsilon_{eq}^{pl}).$$

where $\varepsilon_{eq}^{pl}$ is the equivalent plastic strain and $\sigma_p(\varepsilon_{eq}^{pl})$ is the yield function determined based on an experimental stress-strain curve. In order to simulate the failure response of an SVE, we substitute the macroscopic stress tensor $\sigma_M$ with an effective stress tensor $\sigma_{eff}$ as de Souza Neto et al. (2011)

$$\sigma_{eff} = \frac{\sigma_M}{1 - \omega},$$

where $0 \leq \omega \leq 1$ is a scalar parameter characterizing the magnitude of damage, with 0 and 1 indicating the intact and fully damaged stages of the material, respectively. The damage initiates when $\varepsilon_{eq}^{pl}$ reaches a threshold value, $\varepsilon_{th}^{pl}$, which is a function of the equivalent plastic strain rate $\dot{\varepsilon}_{eq}^{pl}$ and the stress triaxiality $\eta = -p/\sigma_{YM}$, where $p$ is the hydrostatic stress and $\sigma_{YM}$ is the effective von-Mises stress (see Hooputra et al. (2004) for different functional forms of $\dot{\varepsilon}_{eq}^{pl}$). Note that using $\eta$ as one of the damage initiation criteria allows for distinguishing between different failure modes under tensile and compressive loads (i.e., brittle versus ductile failure, respectively). An internal state variable $\omega_{inf}$ is defined as

$$\omega_{inf} = \int \frac{d\varepsilon_{eq}^{pl}}{\dot{\varepsilon}_{eq}^{pl}(\eta, \varepsilon_{eq}^{pl})},$$

for which a unity value ($\omega_{inf} = 1$) indicates the initiation of damage at a given point within the epoxy matrix. After detecting the damage initiation, it is assumed that $\omega = \omega(\bar{\varepsilon}_{eq}^{pl})$ is monotonically increasing from 0 to 1 as an exponential function of the effective plastic displacement $\bar{\varepsilon}_{eq}^{pl}$, the rate of which is given by Hooputra et al. (2004)

$$\bar{\varepsilon}_{eq}^{pl} = L \dot{\varepsilon}_{eq}^{pl}.$$
requires taking into account the interfacial damage between embedded carbon fibers and the surrounding epoxy matrix. We simulate this process by combining a cohesive zone model (CZM) (Safaei et al., 2015; Miniccino and Santare, 2012) with a surface-based contact model (Park and Paulino, 2012). The former simulates the fiber-matrix debonding process, while the latter is utilized to avoid an unrealistic interpenetration between fibers and the matrix after debonding. In the CZM used in this work, a cohesive stiffness tensor $K$ is employed to correlate the traction vector $t$ to the contact-separation vector $\delta$ as

$$\begin{bmatrix}
    t_x \\
    t_y \\
    t_z
\end{bmatrix} =
\begin{bmatrix}
    K_{xx} & 0 & 0 \\
    0 & K_{yy} & 0 \\
    0 & 0 & K_{zz}
\end{bmatrix}
\begin{bmatrix}
    \delta_x \\
    \delta_y \\
    \delta_z
\end{bmatrix}.
$$

(11)

In this traction-separation law, vector/tensor components $\square_x$ and $\square_y$ refer to two orthogonal shear components, while $\square_z$ indicates normal component.

Defining $t_0^x$ and $t_0^y$ as shear strengths and $t_0^z$ as the normal strength along fiber-matrix interface, the damage initiation criterion is given by

$$
\max\left(\frac{t_x}{t_0^x}, \frac{t_y}{t_0^y}, \frac{t_z}{t_0^z}\right) = 1.
$$

(12)

According to the equation above, both shear and normal components of traction, whichever reaches the maximum first, could lead to the initiation of damage along material interfaces. However, using the Macaulay brackets in $(t_0)$ indicates that only tensile normal tractions contribute to this process and compressive tractions have no effect on the initiation of damage (handled using the contact model). Once the criterion given in (12) is satisfied, the propagation of interfacial damage is simulated by degrading the cohesive stiffness tensor $K$ as

$$
t = (1 - D)K \delta.
$$

(13)

where $0 \leq D \leq 1$ is a scalar damage parameter ($0$: no damage; $1$: fully damaged). We use a bilinear law to evaluate the evolution of $D$ as

$$
D = \frac{\delta_1}{\delta_{\text{max}}} - \frac{\delta_2}{\delta_{\text{max}}}.
$$

(14)

where $\delta_1$, $\delta_{\text{max}}$, and $\delta_2$ are the damage initiation separation, maximum effective separation, and complete failure separation along the interface.

When the normal component of the separation vector $\delta$ becomes negative, a contact model is utilized to avoid the matrix-fiber interpenetration. The contact condition is defined by a hard over-closure relation, where the tangential component of $\delta$ is evaluated by enforcing $\delta_n = 0$. This can be achieved by incorporating constraint equations through either Lagrange multipliers (Carpenter et al., 1991) or penalty methods (Park and Paulino, 2012). In this study, it is assumed that $\delta_n$ is enforced to remain zero after surface contact using the penalty approach as Park and Paulino (2012)

$$
t_n = K_p \delta_n.
$$

(15)

where $K_p$ is the penalty stiffness that has a relatively large value at the zero separation. More implementation details regarding this contact model are presented in Park and Paulino (2012).

3. Resin-rich zones and microstructural uncertainty

An SEM image of the CFRP microstructure studied in this work is illustrated in Fig. 1. Unlike aerospace-grade CFRPs reinforced with fibers that have circular cross sections and relatively similar diameters, embedded fibers in this composite material fabricated for automotive applications have oval-shaped cross-sections and a large variation in diameters. In a recent article (Ahmadian et al., 2019), the authors studied the effect of shape and size distribution of these fibers compared to circular-shaped fibers, as well as random small-angle fiber misalignments, on the failure response. The current work aims to shed light on the impact of another important microstructural feature on the mechanical behavior of this CFRP: The presence of large (relative to size of fibers) resin-rich zones with various shapes and sizes in each ply (cf. Fig. 1a). This feature is an artifact of the low-cost manufacturing process employed to provide an economic picture that justifies the application of this CFRP in the automotive industry. As shown in Fig. 1, each CFRP ply is formed by laying multiple fiber bundles side-by-side, each of which consisting of hundreds of fibers. Large resin-rich zones form due to the lack of perfect integration between these bundles during the resin infusion. Smaller resin-rich zones could also form within each bundle and in particular near with their top/bottom edges (adjacent to neighboring plies) due to the relocation of fibers during the manufacturing process.

A hypothetical RVE that can statistically capture the shapes, sizes, and spatial arrangement of resin-rich zones and thus their impact on homogenized properties of each ply of CFRP depicted in Fig. 1 must have a very long in-plane length compared to its width (i.e., the thickness of that ply). This high length-to-width ratio, where the former would be in the order of several millimeters, leads to two major challenges that prohibit performing a CH-based micromechanical analysis. The most severe challenge is that characteristic length scales of such RVE violates the basic requirement of principle of separation of scales in the CH formulation. In other

![Fig. 1. SEM image of a cross-ply CFRP microstructure with embedded oval-shaped fibers: (a) arrangement of fibers in each ply, showing fiber bundles and resin rich zones; (b) larger view of the red inbox shown in figure a, illustrating the shape, size distribution, and spatial arrangement of fibers. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](https://doi.org/10.1016/j.ijsolstr.2019.10.004)
words, we can no longer overlook the variation of macroscopic stresses/strains in an RVE with a length of several millimeters; meaning an RVE does not in fact exist in this case. This is a corollary of the presence of two distinct sub-scales within CFRP lamina; oval-shaped fibers with small relative distances versus considerably larger resin-rich zones scattered over a much wider length. Even if one overlooks this fact, which leads to a significant error, it is still practically impossible to simulate the failure response of such a large (hypothetical) RVE consisting of thousands of fibers. Even in 2D, a corresponding high fidelity FE model would have an exceedingly large number of degrees of freedom, which leads to a huge computational cost. More importantly, it would not be feasible to achieve numerical convergence in such a massive nonlinear problem, involving ductile matrix damage, cohesive debonding, and contact along material interfaces.

To address the challenges outlined above, we create three large SVEs of the CFRP microstructure with different shapes, sizes, and distributions of resin-rich zones. Each virtually reconstructed SVE replicates the distribution of resin-rich zones in an observation window corresponding to a different CFRP ply, although not large enough to statistically represent their dispersion in the whole microstructure. High fidelity FE simulations are then carried out to shed light on the impact of resin-rich zones on the failure response of these SVEs subject to transverse tension, compression, and shear loads. It is worth mentioning that the size of virtual SVEs could affect their homogenized stress-strain responses, as they are not representative of the entire CFRP ply microstructure. However, given the difference between shapes, sizes, and spatial arrangement of resin-rich zones of, their average failure responses would be a good indication of macroscopic mechanical properties of CFRP plies while also shedding light on scattering in mechanical properties. Note that we have only studied three SVEs in this work, as corresponding damage simulations were computationally demanding and even the construction of FE models was not feasible without the implementation of a parallel mesh generation algorithm (i.e., parallel CISAMR Liang et al. (2018)).

4. Modeling process

4.1. High-fidelity micromechanical modeling

In this section, we describe the automated computational framework implemented for creating high fidelity FE models of CFRP SVEs, involving the microstructure reconstruction (Yang et al., 2018) and mesh generation (Nagarajan and Soghrati, 2018) algorithms. Although we have modified the former to reconstruct SVEs with resin-rich zones, a similar framework was recently used in Ahmadian et al. (2019) to analyze the impact of fibers misalignment and their cross-sectional geometry on the failure response of CFRP. For completeness, here we provide a brief overview of this reconstruction algorithm, as well as the modifications made to synthesize SVEs with resin-rich zones.

The process of reconstructing virtual SVEs based on SEM images of the CFRP is schematically shown in Fig. 2. After performing required image processing steps such as the noise filtration, smoothing, binarization, and segmentation (cf. Fig. 2a), we extract morphologies of a representative set of fibers and store them in a shape library. The cross-section of each oval-shaped fiber in this library is characterized using a Non-Uniform Rational B-Spline (NURBS) curve Yang et al. (2018). In addition to shapes of fibers, we also extract three statistical microstructural descriptors from the imaging data, namely the volume fraction of fibers, their size distribution (log-normal probability distribution function), and spatial arrangement (two-point correlation function Yang et al., 2018). For the latter, we extract and average this probability distribution function from multiple small region of the SEM image without large resin-rich zones, e.g., the region illustrated in Fig. 1b. A separate shape library and similar statistical microstructural

![Fig. 2. Different steps of the algorithm used for the image-based virtual reconstruction of CFRP SVEs with resin-rich zones.](image-url)
descriptors are also extracted for resin-rich zones observed in CFRP plies (cf. Fig. 1a) to replicate them in final synthesized SVEs.

In order to virtually reconstruct an SVE, we initially overlook the presence of resin-rich zones in the CFRP microstructure. The algorithm used for this purpose consists of two main phases, starting with virtually packing fibers within the SVE domain to build an initial (raw) microstructure. The targeted volume fraction of fibers in these raw microstructures is $V^\text{raw} = 55\%$, which is on average 5% higher than the targeted volume fraction of final SVEs with resin-rich zones. Until reaching $V^\text{raw}$, we pick a fiber from the shape library and apply a scale factor to that based on the probability distribution function associated with the size of fibers. This new fiber is then rotated at a random angle and a random location within the SVE domain is assigned to that. As shown in Fig. 2b, we then employ a set of hierarchical bounding boxes (BBoxes) to detect/eliminate overlaps between new and existing fibers. This process involves the following three main steps:

1. Check intersection between the enlarged BBox of the new fiber and primary BBoxes of existing (previously added) fibers to identify those in its close proximity of this new fiber. A quadtree search algorithm is used in this step to enhance the search process. In Fig. 2c, this computationally-expensive, heuristic check identifies fibers 3 and 6 as those potentially overlapping with the new fiber.

2. Check intersection between the primary BBox of the new fiber with those of the existing fibers identified in first step to further eliminate non-overlapping fibers. In Fig. 2c, this check rules out the possibility of overlap between fiber 6 and the new fiber.

3. Check intersection between secondary BBoxes of the existing fibers not excluded after the completion of the second step (e.g., fiber 3 in Fig. 2c) and secondary BBoxes of new particles to more precisely determine if they overlap with one other or not. No overlap means the new fiber can be added to SVE. Otherwise, we can move the new fiber horizontally or vertically to edges of its enlarged BBox (four possible directions), redo the checks in steps 2 and 3 to determine if we can insert it at one of these locations. If still not feasible, a new random location must be assigned to the new fiber and the whole process restarted.

The second phase of reconstructing a realistic SVE without resin-rich zones is to modify the virtually packed microstructure to replicate the target two-point correlation function associated with the spatial arrangement of fibers. To achieve this, we define an optimization problem with the objective of minimizing the $L_2$-norm of the error, $e_2$, between the initial and target two-point correlation functions. The initial microstructure is then evolved into an optimized SVE with the desired spatial arrangement of fibers using the Genetic Algorithm (GA), during which fibers are either relocated within their enlarged BBoxes or eliminated to minimize $e_2$ (cf. Fig. 2d). Although GA is often regarded as a computationally expensive evolutionary algorithm, here we could reach $e_2 < 1\%$ in less than 20 generations with an initial random population with the size of 100. More details regarding the optimization phase are presented in Yang et al. (2018).

In order to build the final SVE, we first employ the packing-optimization algorithm described above to build a model with similar dimensions as the SVEs composed of only resin-rich zones. Note that the shape and size distributions of these regions are determined based on the corresponding shape library and log-normal distribution function extracted from SEM images. As shown in Fig. 2d, the SVE microstructure obtained from the packing-optimization process described previously is then overlaid with resulting resin-rich zones and any underlying fiber fully confined within one of these zones is eliminated with a probability of 98%.

Fig. 3 illustrates three $750 \mu m \times 170 \mu m$ SVEs virtually constructed using this combined algorithm, in which volume fractions of fibers could be different due to the variation in the cumulative areas of resin-rich zones. Here, SVE-A has the lowest fibers volume fraction ($V_f \approx 49.1\%$), while for SVE-B and SVE-C the volume fractions are $V_f \approx 50.2\%$ and 51.3\%, respectively. It is worth mentioning that although the reconstruction algorithm described above can easily create periodic microstructures, which in turn enables the use of periodic BC in FE models, we have deliberately not utilized this feature in the current study. This is due to the geometrical

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Fig. 3. Virtually reconstructed principal SVEs of the CFRP with different spatial arrangements of fibers and slightly different volume fractions. SVE-A: $V_f = 49.1\%$; SVE-B: $V_f = 50.2\%$; and SVE-C: $V_f = 51.3\%$.

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feature and large size of resin-rich zones, scattered at large distances throughout each SVE, for which using the assumption of periodicity is rather unrealistic. Further, because each CFRP ply is confined within two cross-ply axes along its top and bottom edges, the use of periodic BC along them is not physically realistic.

Finally, the virtually reconstructed SVEs are transformed into high fidelity FE models using the CISAMR mesh generation algorithm (Soghrati et al., 2017; Nagarajan and Soghrati, 2018). In 2D, CISAMR transforms a background structured mesh composed of quadrilateral elements into a hybrid mesh (quadrilateral and triangular elements) that conforms to material interfaces using a non-interactive algorithm consisting of h-adaptivity, r-adaptivity, and sub-triangulation phases. In this work, cohesive elements are also created along material interfaces to simulate the fiber-matrix debonding during the failure analysis. Fig. 4 shows small portions of the conforming mesh constructed using this algorithm corresponding to the inboxes shown in Fig. 3 for SVE–A. Given the large size of meshes built for principal SVEs in this work (e.g., 1.82 million elements and 8.15 million degrees of freedom for SVE–A), we have implemented CISAMR in parallel to generate these meshes (Liang et al., 2018).

5. High-fidelity failure analysis

5.1. Material properties

In this section, we use the high-fidelity FE models of SVEs to predict their failure response subject to loadings applied in the transverse fibers direction. In the plane strain simulations presented next, it is assumed that the epoxy matrix has an elastic modulus of $E_m = 3$ GPa and a Poisson’s ratio of $\nu = 0.35$, while both carbon fibers are $E_c = 23$ GPa and $\nu_{cf} = 0.445$. Note that although carbon fibers are transversely isotropic, as shown in Ahmadian et al. (2017), their longitudinal stiffness does not affect the CFRP failure response subject to loadings applied in the transverse fiber direction. The parameters used in the continuum ductile damage model for this phase are calibrated with experimental stress-strain curves obtained from tension, compression, and shear tests on pure epoxy specimens (Fiedler et al., 2001; Au and Büyükoğrüz, 2006). Table 1 shows the calibrated stress-strain data used in the plastic yield function $\sigma_y (\varepsilon_{pl}^0)$. The calibrated thresholds for equivalent plastic strains before the damage initiation under tension, compression, and shear are $\varepsilon_{pl}^0 = 0.033$, 0.13, and 0.27, respectively. Also, the material can sustain effective plastic strains $\bar{\varepsilon}_{pl} = 0.01 \mu m$, 0.1 $\mu m$, and 0.2 $\mu m$ before failure subject to tensile, compressive, and shear loads, respectively (Liang et al., 2019).

For the cohesive damage model adopted to simulate the fiber-matrix debonding, the cohesive stiffness and strength values are $K_a = K_s = K_t = 4.54$ GPa and $t_0 = t_0^c = t_0^t = 33.5$ MPa, while the effective separation after damage initiation is $\delta_{pl} = 0.5 \mu m$. These parameters are calibrated with experimental peel tests and molecular dynamics (MD) simulations presented in Lau et al. (2012) and de Almeida and Neto (1994), where the latter takes into account the impact of hydrogen bonds on the epoxy–carbon interfacial strength (Horie et al., 1976). More details regarding the calibration of parameters used in the continuum and interfacial damage models are presented in Ahmadian et al. (2019).

5.2. Effect of loading type

The damage patterns in the SVEs subject to different loadings applied in the transverse fibers direction (tension and compression along y axis, as well as transverse shear) are illustrated in Figs. 5–7. As shown in these Figures, main damage paths (major cracks) in none of the SVEs and under none of the loading conditions passes through the resin-rich zones. Instead, the damage often nucleates and propagates in regions of fiber clustering, as stress concentrations are amplified in such areas due to the close proximity of fibers Totry et al. (2008b) and Vaughan and McCarthy (2011). This feature is especially evident in Fig. 7 for SVE–C. Note that while embedded fibers reinforce CFRP in the longitudinal fibers direction, they practically act as sites of stress concentrations subject to transverse loads. A combination of high stress concentrations and the weak bonding along fiber-matrix interfaces accelerates the damage initiation in such regions. In contrast, although resin-rich zones can highly deteriorate the longitudinal strength of CFRP, they are immune to such damage mechanisms under transverse loading. For example, as shown in Fig. 6a, the major crack under tension is significantly deviated from its path near the resin-rich zone in SVE–B to bypass this region.

The resulting macroscopic stress-strain responses of SVEs subject to different loading conditions are presented in Fig. 8. As shown in this figure, a semi-brittle failure response is observed under tension, while all SVEs exhibit moderate and significant ductile behaviors subject to compressive and shear loads, respectively. Although the increase in fibers volume fraction from SVE–A to SVE–C is insignificant (from 49.1% to 51.3%), a notable increase is observed in corresponding failure strains under a tensile load. This

### Table 1

<table>
<thead>
<tr>
<th>$\sigma_y$ (MPa)</th>
<th>29.0</th>
<th>37.0</th>
<th>52.2</th>
<th>84.8</th>
<th>95.3</th>
<th>96.3</th>
<th>97.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{pl}^0$</td>
<td>0.0</td>
<td>4.95e-4</td>
<td>1.50e-3</td>
<td>1.01e-2</td>
<td>2.27e-2</td>
<td>2.72e-2</td>
<td>1.42e-1</td>
</tr>
</tbody>
</table>

is due to the toughening mechanism provided by carbon fibers, which strengthen and prolong the failure process. On the other hand, it is evident in Fig. 8 that the SVE with the least fibers volume fraction (i.e., SVE–A) has the highest strength and toughness. Note that a higher volume fraction of fibers in SVE–B and SVE–C indicates an average smaller spacing between fibers. Further, the presence of larger resin-rich zones in these SVEs leads to a higher chance of fiber clustering away from these regions, which in turn accelerates the damage nucleation and its growth. Thus, the more uniform spatial arrangement of fibers in SVE–A compared to these SVEs leads to a higher strength and toughness, despite its lower ductility. These observations are consistent with the results of the study presented in Naya et al. (2019). It is worth mentioning that the plateau region after the initial softening in macroscopic stress-strain responses of SVEs under tension (cf. Fig. 8a) is merely a numerical artifact, meaning the transition between them can be regarded as the failure point.

The damage patterns formed in SVEs subject to a compressive load (e.g., Fig. 5b) also show the concentration of damage in regions with a smaller fiber spacing and away from resin-rich zones. For this loading condition, the shear bands developed in the matrix form an average angle of 45° with the loading direction, which is compatible with the experimental and numerical observations reported in Naya et al. (2017) and Chevalier et al. (2019a). The damage patterns shown in Fig. 9 also demonstrate the ability of the FE model to handle contact between fiber-matrix and fiber-fiber while simulating the matrix crushing and shear band formation under this type of loading. As shown in Fig. 8b, in contrary to the case of tensile load, here the strength and toughness of SVE–C (highest volume fraction) are higher than those of the other two

SVEs. In this case, after the fiber-matrix interfacial cohesive failure due to the formation of highly localized tensile and shear stresses around fibers, the isolated matrix entrapped between fibers can still maintain a linear elastic behavior while increasing the compressive load. After a significant plastic deformation and finally the damage evolution, this region of the matrix crushes, which leads to collision between adjacent fibers. When this phenomenon occurs, the CFRP strength locally increases until shear bands coalesce to form the criss-cross damage pattern shown in Figs. 5b–7b. Thus, a higher volume fraction of fibers under compression means that a larger number of fibers contribute to transferring the applied load through contact after the crushing of surrounding matrix, which in turn provides a higher compressive strength. This damage mechanism leads to strain hardening phase in the macroscopic stress-strain response, followed by a steady exponential reduction in stiffness and thereby a more ductile behavior compared to the case of

tensile loading. It is worth mentioning that under compression, the large resin-rich zones in SVE-B and SVE-C undergo a significant amount of plastic deformation without experiencing damage.

Despite the variation in the volume fraction and spatial arrangement of fibers, as shown in Fig. 8a, failure response of all three SVEs are nearly identical under a transverse shear loading. Note that under shear, hydrostatic tensile stresses and subsequently triaxial values along fiber-matrix interfaces are not significant. Therefore, the damage nucleation in these regions is considerably less than that observed subject to compressive and tensile loads; thus that the softening response of the matrix is counteracted by plastic hardening. Subsequently, no clear softening behavior or strength drop is observed in the macroscopic stress-strain response of the CFRP under transverse shear (cf. Fig. 8a).

In addition to the spatial arrangement of fibers in each SVE, the orientation of oval-shaped fibers affects the damage path in this CFRP. This is due to higher stress concentrations developed in fiber-matrix interfacial regions with higher curvatures, which enhances their deboning followed by the nucleation of damage in the surrounding matrix. For example, the initiation of damage and plastic deformation under compression is caused by the punching of fibers to the matrix, which is magnified when longer radii of fibers are aligned with the loading direction. This observation is consistent with the results of a recent numerical study on the effect of fiber shape on the transverse strength of unidirectional CFPRs Herráez et al. (2016). However, given the large size of the SVEs studied in this work, assigning random fiber orientations and similar probability distribution functions for their radii in the reconstruction algorithm leads to statistically equivalent microstructural models. In other words, the main microstructural descriptor that sets these SVEs apart is the spatial arrangement of fibers, which in turn is governed by how resin-rich zones are distributed within each SVE. Therefore, since the volume fractions of fibers in the SVEs are not significantly different, the variation observed in their failure responses (strength and toughness) are mainly attributed to the difference in local clustering of fibers in each model.

5.3. Effect of loading direction and BC

Since the length-to-width ratio of the SVEs studied in this work is approximately 4.4, we have analyzed their failure responses subjected to transverse tensile and compressive loads in the x direction to compare them to previous results considering loadings in the y direction. Note that for each simulation, displacement BC is assigned along the SVE edges perpendicular to the loading direction (e.g., top and bottom edges for tension in the y direction), while the parallel boundaries are considered traction free.

As shown in Fig. 10, a negligible difference is observed between resulting macroscopic stress-strain curves when a tensile load is applied in either of these directions. This is due to the statistical equivalency of SVEs in both directions, as resin-rich zones of both SVEs (despite differences in their orientations in the x and y direction) are immune to the damage nucleation. Therefore, since the spatial arrangement of fibers is statistically equivalent in both directions (orientation, spacing, etc.) and failure under tension is caused by one major crack path, the SVEs show similar failure responses in both directions.

The macroscopic stress-strain response of SVEs under compression in the x and y directions (cf. Fig. 10) show a completely different behavior, which contradicts the argument provided previously for the case of tensile loading. First, we study the behavior of SVEs with the traction free BC is assigned along both top and bottom edges when the compressive load is applied in the x direction. Compared to the macroscopic stress-strain responses of SVEs subject to compression in the y direction, less ductility and a significant reduction in strength (e.g., 32% for SVE-A) are observed. The damage patterns in SVEs under compression in the x direction and with two traction free edges are illustrated in Fig. 11. Unlike the SVEs subject to a compressive load in the y direction (Figs. 5–7), in this case, the formation of a single shear band leads to failure. Here, the traction free BC along the top and bottom edges and the small width of the SVE relative to its length facilitate the sliding of the segments on opposing sides of the shear band under the compression in the x direction, causing the immediate instability and failure. Therefore, in the absence of constraints along these edges, the small width-to-length ratio (slenderness) of the SVE accelerates this buckling-like failure mode. Note that among the three SVEs loaded under compression in the x direction, SVE-A shows the least strength and ductility. The cause of this behavior is similar to that explained previously for the compression in the y direction, where the lower volume fraction of fibers and smaller resin-rich zones in SVE-A compared to those in SVE-B and SVE-C accelerates the formation of shear bands.

In practice, a single ply of CFRP is never used as a structural component and therefore the assumption of assigning traction free BC along both the top and bottom edges of an SVE loaded in the x direction is rather unrealistic. Yet, the study presented in the paragraph above shows the crucial effects of size and BC of SVEs on their failure response under compression. Yet, there is another case scenarios that assigning the traction free BC along only either the top or the bottom edge of an SVE under compression is not only realistic but also essential when the loading is applied in the x direction. For example, consider an SVE corresponding to the bottom laminate of a cross-ply CFRP. Subject to loadings applied in the transverse fiber direction, the bottom edge of this SVE must
be modeled as a traction free boundary. On the other hand, because another CFRP ply with the fibers oriented perpendicular to those in this ply (cf. Fig. 1a) constrains the deformation along the top edge, as an upper bound, we can fix the displacement DOFs in the y direction along this edge. In reality, the upper ply is also compliant and could experience damage, meaning that in a more realistic FE analysis the cross-ply must also be incorporated in the model. However, given the exceedingly high computational cost of creating such large cross-ply SVEs in 3D, this model could yield an upper bound for the strength of such plies.

The macroscopic stress-strain responses of supported SVEs (fixed along the top edge, traction free along the bottom edge) under compression in the x direction are illustrated in Fig. 10. As shown in this figure, compared to SVEs with two free BCs subject to the compression in the same direction, an average increase of 10% is observed in the strength. However, compared to the case of loading in the y direction, the strength has a notable average decrease of 17%. Similarly, the ductility of supported SVEs is more than the case of compression in the x direction with two free BCs but less that of the compression in the y-direction. Simulated...
damage patterns in supported SVEs is illustrated in Fig. 12, where still a single major shear band has led to failure. However, compared to the simulation under compression in the x direction with two free BCs, only the damage pattern in SVE–C is rather identical. Here, the additional constraint imposed on the upper edge of the SVEs makes the formation of shear band more difficult by resisting the sliding of SVE segments on each side of the crack. Note that for all three types of simulations under compression (y dir.; x dir., free BC; x dir., fixed top), SVE–A that has the smallest resin-rich zones consistently yields a lower strength than the other two SVEs.

The study above shows the impact of the traction free edge of SVEs corresponding to top/bottom lamina of a cross-ply CFRP in reducing their compressive strength in the x-direction compared to that of the y-direction. It is worth mentioning that using fixed BC along both the top and bottom edges of an SVE loaded under compression in the x direction prohibits the material failure. This assumption is realistic for internal plies of a cross-ply composite provided that we assume the supportive plies on the top and bottom (which are loaded in the longitudinal fibers direction) do not fail. In this case, as shown in Fig. 13, the damage locally nucleates in regions with highly clustered fibers due to crushing of the surrounding matrix. However, the supportive plies do not allow the formation of shear bands, as CFRP segments on either side can no longer slide relative to one another. In the FE simulation, this eventually leads to convergence difficulties, as over-constraining the domain does not allow transitioning to the softening response in stress-strain curve (cf. Fig. 10). Simultaneously, the increased stress triaxiality in the domain makes the matrix crushing more difficult and even after that fiber-fiber contact maintains the load bearing capacity of SVE. Note that the supportive cross-lamina on the top and bottom finally experience failure by increasing the compressive load (often due to fiber buckling), which eventually allows the formation of shear bands and failure of this ply.

6. Conclusion

An integrated computational framework relying on high fidelity FE simulations was implemented to study the failure response of a CFRP with large resin-rich zones under tensile, compressive, and shear loads applied in the transverse fibers direction. The modeling process involved the use of a packing-optimization algorithm to reconstruct three realistic SVEs of CFRP, each with different size and spatial arrangement of resin-rich zones. The CISMAR non-iterative meshing algorithm was then employed in parallel to generate high-quality, adaptively refined conforming meshes composed of millions of elements for each SVE. The FE approximations of failure response of SVEs were carried out using continuum ductile and cohesive-contact damage models for the epoxy matrix and fiber-matrix interfaces, respectively. Main outcomes of the study are summarized below:

- While resin-rich zones are immune to damage nucleation under transverse loads, the accompanied fiber clustering away from these regions accelerates the damage initiation in SVEs.
- Presence of large resin-rich zones in the matrix leads to a reduction in strength under tension, no meaningful impact on the failure response under transverse shear, and an increase in strength under compression.
- Despite the large length (along x axis) to width (along y axis) ratio of SVEs of each ply, the BC used in the FE model has a negligible impact on the failure response when a tensile load is applied in either x or y directions.
- In contrary, the boundary conditions highly affect the simulated strength of SVEs under compression, specially when the loading is in the x-direction (parallel to the ply). It was shown that applying traction free BC on one of the edges, which correspond to SVEs from either one of the top or bottom lamina of a cross-ply CFRP leads to a notable decrease in the strength.

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References


Fig. 13. Damage pattern in the final converged solution for SVE-B with both top and bottom edges fixed subject to a compression in the x-direction (see Fig. 10 for the corresponding macroscopic stress-strain response).