Numerical prediction of uniaxial tensile properties of 3D braided C/SiC composites

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Abstract. This paper is focused on the microstructure modeling and numerical prediction of uniaxial tensile properties of three-dimensional (3D) braided carbon fiber-reinforced silicon carbide (C/SiC) composites. Based on the multiscale characteristics of the fabrication process and component material distribution of 3D braided C/SiC composites, fibre scale and tow scale RVE models were established considering the local periodicity of the microstructure of the composites. Finite element method was applied to predict the elastic properties and strength properties of the fibre scale model, which were then substituted into the tow scale model. The Tsai-Wu failure criterion was employed and the stiffness reduction was conducted in the failed elements according to the different failure modes. The progressive damage process of 3D braided C/SiC composites under uniaxial tensile load was simulated.

1. Introduction
Three-dimensional (3D) braided composites are a new type of reticulated structure composites. Because of the one-time braiding of preforms, the 3D integral reticulated structure is formed by fibers passing through the three directions of length, width and height. Therefore, the problems of low stiffness and strength along thickness direction, low in-plane shear and interlaminar shear strength, easy delamination, low impact toughness and damage tolerance of traditional composite materials are fundamentally solved. 3D braided C/SiC has many advantages, such as high strength, high temperature resistance, low density and high toughness. It has broad application prospects in aerospace field[1-4].
In order to determine the mechanical properties of 3D braided composites, various models and strategies have been proposed[5-8]. The research on mechanical properties of 3D braided C/SiC composites is mainly focused on experimental analysis and theoretical calculation. Calard et al.[9] studied the statistical distribution of ceramic matrix composites and proposed a macro probability model to predict the final failure. Wang et al.[10] applied acoustic emission technology to analysis the damage of braided ceramic matrix composites.
In this paper, a numerical method is presented to predict the uniaxial tensile properties of a 3D braided C/SiC composite [11]. Firstly, the elastic constants and strength properties of the fibre scale model are predicted by finite element method. Then these parameters are substituted into the tow scale model. Considering the different damage modes of fiber bundles, the uniaxial tensile properties of 3D braided C/SiC composites are obtained numerically. The simulation results are in good agreement with the experiment data.

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2. Multiscale microstructure modeling strategy

The RVE model of the 3D braided composite involves two scales: the first scale concerns the modelling of RVE for tows and second scale concerns the modelling of RVE for 3D four-step braided composites. Considering the multiscale characteristics of the model, a multiscale analysis method[12-14] is applied to the analysis of braided composites. The process of multiscale analysis is as follows. Firstly, on the fibre scale, finite element model is built to obtain the equivalent moduli and strength properties in all directions of the fibre scale RVE, and the results are used for the tows that were treated as a homogeneous transversely isotropic material. Secondly, based on the obtained elastic and strength properties of tows, finite element model of the tow scale RVE is built to evaluate effective elastic properties and uniaxial tensile properties of the composite. Here, RVE models of both scales are established in finite element software ANSYS.

2.1. Fibre scale model

Tows can be regarded as unidirectional composites with uniform fiber accumulation and distribution. Square and hexagonal accumulation are common fiber accumulation modes. As seen in figure 1, fibers accumulate in regular hexagonal shape, and the PyC interphase and SiC matrix are distributed around the fibres (different colours represent different material phases). Characteristic geometric parameters of the RVE model are fibre diameter $\phi_i$ and thicknesses of the PyC interphase $T_v$. The finite element model of the RVE is depicted in figure 1. where 8-node prismatic solid element SOLID5 of ANSYS software is used.

![Figure 1](image1.png)

**Figure 1.** RVE model on fibre scale (a) Characteristic geometric parameters, (b) Finite element model of fibre scale RVE.

2.2. Tow scale model

In tow scale, the RVE model of the 3D braided composite is established. The RVE model used in this paper is followed from which described in our past work: the cross-section of tow is hexagonal; the braided structure is uniform and all the tows are straight within the braided preform; all tows in the braided preform have identical constituent material, size and flexibility. More details about the geometry of the RVE can be found in [15].

Figure 2 shows the tow scale RVE model of a $22^\circ$ braiding angle. The finite element model of the RVE is depicted in figure 5b where 8-node prismatic solid element SOLID5 of ANSYS software is used.

![Figure 2](image2.png)

**Figure 2.** RVE model on tow scale (a) geometrical model, (b) finite element model
3. Computation methods of elastic constants and strength properties on fibre scale

3.1. Strain energy-based approach

In this study, a strain energy-based finite element approach is applied to evaluate effective elastic properties with specific boundary conditions imposed on the RVE. The detailed description of this method can be found in our previous studies. Here, only a basic introduction is presented. In the elastic regime, the macroscopic behaviors of the RVE can be characterized by the effective stress tensor $\overline{\sigma}$ and strain tensor $\overline{\varepsilon}$. They are interrelated by the effective, also termed homogenized, stiffness matrix $C^H$.

$$\overline{\sigma} = C^H \overline{\varepsilon}$$

(1)

where $\overline{\sigma} = \frac{1}{V} \int_{\Omega} \sigma d\Omega$, $\overline{\varepsilon} = \frac{1}{V} \int_{\Omega} \varepsilon d\Omega$ and $V$ is the volume of the RVE.

Consider the case of 3-D orthotropic materials, equation (3) corresponds to

$$C^H = \begin{bmatrix}
C_{111}^H & C_{112}^H & C_{113}^H & 0 & 0 & 0 \\
C_{112}^H & C_{222}^H & C_{223}^H & 0 & 0 & 0 \\
C_{113}^H & C_{223}^H & C_{333}^H & 0 & 0 & 0 \\
0 & 0 & 0 & C_{122}^H & 0 & 0 \\
0 & 0 & 0 & 0 & C_{223}^H & 0 \\
0 & 0 & 0 & 0 & 0 & C_{333}^H
\end{bmatrix}$$

(2)

The strain energy related to the RVE is equal to:

$$E = \frac{1}{2V} \left( \sigma_{11} \varepsilon_{11} + \sigma_{22} \varepsilon_{22} + \sigma_{33} \varepsilon_{33} + \sigma_{12} \varepsilon_{12} + \sigma_{23} \varepsilon_{23} + \sigma_{31} \varepsilon_{31} \right) d\Omega$$

(3)

With the help of specific boundary conditions, the combination of equation (2) and equation (3) can be used to deduce the effective stiffness matrix $C^H$ for the RVE. Suppose a unit initial strain is imposed in the direction 1, i.e. $\overline{\varepsilon}^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T$. Note that the superscript $(1)$ represents the first load case. The corresponding average stress is then obtained by equation (2):

$$\overline{\sigma}^{(1)} = \begin{bmatrix} C_{111}^H & C_{112}^H & C_{113}^H & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T$$

(4)

By replacing $\overline{\sigma}^{(1)}$ and $\overline{\varepsilon}^{(1)}$ into equation (3), one obtains the following expression of the strain energy:

$$E^{(1)} = \frac{1}{2} \overline{\sigma}^{(1)} \overline{\varepsilon}^{(1)} V = \frac{1}{2} C_{111}^H V$$

(5)

The matrix coefficient $C_{111}^H$ can be derived:

$$C_{111}^H = \frac{2E^{(1)}}{V}$$

(6)

In the same way, demonstrations can be made for other coefficients. The elastic properties can be further derived by inverting the elastic matrix. In practice, the considered RVE will be discretized into a finite element model on which the initial strain will be imposed to evaluate the strain energy. Table 1 shows the elastic properties of each component in the C/PyC/SiC model. The equivalent elastic constants of the C/PyC/SiC model are obtained by the above method, as shown in table 2. The predicted material constants are the material properties of the tows in the tow/SiC matrix model. The main direction of the material in the tows is shown in figure 3.
Figure 3. Material orientation inside the yarn.

Table 1 Mechanical properties of component materials

| Component         | Modulus $E_{11}$ (GPa) | Modulus $E_{33}$ (GPa) | Poisson ratio $G_{12}$ (GPa) | Poisson ratio $G_{23}$ (GPa) | Tensile strength $v_{12}$ (MPa) | Compressive strength $v_{23}$ (MPa) | Shear strength $v_{12}$ (GPa) | Shear strength $v_{23}$ (GPa) |
|-------------------|------------------------|------------------------|-----------------------------|-----------------------------|---------------------------------|---------------------------------|------------------------------|------------------------------|
| SiC fiber         | 22.0                   | 220                    | 7.75                        | 4.8                         | 0.42                            | 0.12                            | 3528                         | 2500                         |
| PyC interphase    | 20                     | 30                     | 2                           | 8.13                        | 0.23                            | 0.23                            | 50                           | 50                           |
| SiC               | 350                    | 145.8                  | 0.25                        | 350                         | 0.25                            | 350                             | 3500                         | -                            |

Table 2 Computed results in material properties of fibre scale model

| $E_{11}$ (GPa) | $E_{33}$ (GPa) | $G_{12}$ (GPa) | $G_{23}$ (GPa) | $v_{31}$ |
|----------------|----------------|----------------|----------------|----------|
| 243.8          | 32.2           | 12.4           | 11.0           | 0.11     |

3.2. Periodical boundary conditions

Appropriate boundary conditions can ensure the continuity of displacement and traction at both ends of the micromechanical model, which is very important for obtaining accurate results. Periodic boundary conditions provide a more accurate prediction of effective mechanical properties[16]. Therefore, periodic boundary conditions are selected for micro-mechanical modeling of various loading conditions, including uniaxial tension, compression and shear loading.

Considering the periodic boundary conditions, the displacement field of the RVE model can be expressed by the following equation:

$$ u_i^+ = e_{ij}^x x_j^+ + u_i^* $$

$$ u_i^- = e_{ij}^x x_j^- + u_i^* $$

(7)

In the equation (7), $u_i^*$ is the periodic displacement correction of the boundary; $i$ and $j$ can take three coordinate directions respectively; $e_{ij}$ is the average strain of the RVE; $x_j$ is the coordinate of any point in the RVE; $k^+$ and $k^-$ represent the normal periodic boundary surfaces along the positive and negative directions respectively.

Combining equations (7), the displacement difference between the two opposite boundaries of RVE models is obtained:

$$ u_i^{k+} - u_i^{k-} = e_{ij} (x_j^{k+} - x_j^{k-}) = e_{ij} \Delta x_j $$

(8)

Where, $\Delta x_j$ is a constant of any parallelepiped RVE model. The diagram of periodic boundary conditions under different loading conditions is shown in figure 4. Figure 4(a) shows the original RVE model with three pairs of parallel boundaries. After that, different loading conditions are defined using displacement constraints.
4. Progressive damage analyses

4.1. Failure criteria for fibre scale analysis
Due to the lack of strength data of tows, the finite element method is used to predict the strength values of tows in all directions, which is used in the Tsai-Wu failure criterion. It is generally considered that the matrix is homogeneous isotropic linear elastic material in the conventional use environment. Various strength criteria suitable for isotropic materials can be used to judge the damage of the matrix. For SiC ceramics, the resistance to tensile and compressive damage varies greatly, and the compressive strength is far greater than the tensile strength. Therefore, Mohr's strength theory should be adopted as the strength criterion.

According to different load conditions, periodic boundary conditions are applied to the tow scale RVE. The average stress of the RVE under each load step is calculated by step loading. The strength and final strain of the RVE in each direction are obtained according to the simulated stress-strain curve, as shown in table 3.

| Strength properties of fibre scale RVE in different directions |
|---------------------------------------------------------------|
| **Tensile** | **Compressive** | **Tensile** | **Compressive** | **XY** | **Shear** |
| Strength (MPa) | 31.2 | 956.4 | 2875 | 2202 | 38.9 | 30.5 |
| Strain | 0.0010 | 0.0378 | 0.0153 | 0.0099 | 0.0042 | 0.0041 |

The stress-strain relationship curve fitted by finite element analysis is shown in figure 5. The transverse tensile strength of the model is 31.2 MPa. This is because a pyrolytic carbon interface is deposited outside the fiber, and the strength of the pyrolytic carbon interface is low, which affects the overall transverse tensile strength. Under the axial tensile load, the first step of the model is pyrolytic carbon. The strength failure occurs at the interface and then extends to the SiC matrix, which is ultimately
supported by the SiC fibers. When the SiC fibers reach the strength limit, the material will break in the axial direction. The shear failure of the fiber size model is mainly caused by the interface and matrix cracking, while the fibers remain intact during the failure process.

Figure 5. Stress-strain curves of fibre scale RVE (a) x-direction (b) z-direction (c) xy-direction.

4.2. Failure criteria for tow scale analysis

Due to the complexity of braiding structure, it is not reasonable to adopt the method of stiffness reduction in order to more accurately predict the strength performance of material under specific load conditions. Therefore, it is necessary to improve the specific failure mode of model element. For 3D C/SiC composites, Tsai-Wu failure criterion is introduced into the tow elements, and then the stiffness is reduced according to the tow direction. SiC matrix is usually regarded as isotropic material, and the maximum stress criterion is applied as the failure criterion for the matrix material.

The expression of Tsai-Wu tensor failure criterion is as follows:

$$F_{11}\sigma_{1}^{2} + F_{22}\sigma_{2}^{2} + F_{33}\sigma_{3}^{2} + 2F_{12}\sigma_{1}\sigma_{2} + 2F_{13}\sigma_{1}\sigma_{3} + 2F_{23}\sigma_{2}\sigma_{3} + F_{44}\sigma_{4}^{2} + F_{55}\sigma_{5}^{2} + F_{66}\sigma_{6}^{2} + F_{45}\sigma_{4}\sigma_{5} + F_{46}\sigma_{4}\sigma_{6} + F_{54}\sigma_{5}\sigma_{4} + F_{56}\sigma_{5}\sigma_{6} + F_{64}\sigma_{6}\sigma_{4} + F_{65}\sigma_{6}\sigma_{5} = 1$$

(9)

The strength parameters in Tsai-Wu tensor failure criterion are as follows:

$$F_{11} = 1/(X_{T}X_{C})$$
$$F_{22} = 1/(Y_{T}Y_{C})$$
$$F_{33} = 1/(Z_{T}Z_{C})$$
$$F_{44} = 1/S_{xy}$$
$$F_{55} = 1/S_{xz}$$
$$F_{66} = 1/S_{yz}$$

$$F_{12} = -\frac{1}{2}\left(\frac{1}{X_{T}X_{C}} + \frac{1}{Y_{T}Y_{C}} - \frac{1}{Z_{T}Z_{C}}\right)$$
$$F_{23} = -\frac{1}{2}\left(\frac{1}{Y_{T}Y_{C}} + \frac{1}{Z_{T}Z_{C}} - \frac{1}{X_{T}X_{C}}\right)$$
$$F_{31} = -\frac{1}{2}\left(\frac{1}{Z_{T}Z_{C}} + \frac{1}{Y_{T}Y_{C}} - \frac{1}{X_{T}X_{C}}\right)$$
$$F_{45} = \frac{1}{X_{T}} - \frac{1}{X_{C}}$$
$$F_{54} = \frac{1}{Y_{T}} - \frac{1}{Y_{C}}$$
$$F_{63} = \frac{1}{Z_{T}} - \frac{1}{Z_{C}}$$

(10)

X, Y and Z represent the transverse, normal and axial direction of the tow, T and C represent the tensile strength and compressive strength respectively, and $S_{xy}$, $S_{xz}$ and $S_{yz}$ represent the shear strength. Damage modes $H_{i}$ ($i=1,2$) are specifically defined as:

$$H_{1} = F_{1}\sigma_{1} + F_{3}\sigma_{3}$$
$$H_{2} = F_{1}\sigma_{1} + F_{2}\sigma_{2} + F_{1}\sigma_{1} + F_{2}\sigma_{2} + F_{4}\sigma_{4} + F_{5}\sigma_{5} + F_{6}\sigma_{6}$$

(11)

When Tsai-Wu failure criterion is satisfied, ($i=1,2$) maximum represents the main damage mode. $i = 1$, 2, 3 represents transverse, normal and axial direction of the tow, $i = 4, 5, 6$ represents YZ direction, XZ direction and XY direction respectively.

The maximum stress criterion can be expressed as:
In equation (12), \( X_{\text{int}} \), \( X_{\text{inc}} \), and \( S_{\text{ijm}} \) are the tensile, compressive and shear strengths of the main directions of the matrix respectively.

### 4.3. Damage strategy

When the tow scale model is subjected to step loading, the stiffness matrix of the damaged material based on damage state variables is established by setting different damage modes \( H_i \) (i=1,2) after the element reach the damage criterion. The stiffness of the element is degraded which is shown in equation (13) according to the direction and the constitutive matrix of the element is updated. As the load continues to increase, the failure element is judged in the incremental step simulation, so that the cyclic loading is completed until the analysis is completed. The performance degradation schemes for each component of the material are shown in table 4.

\[
\begin{align*}
\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \tau_{31} \\ \tau_{12} \end{bmatrix} = & \begin{bmatrix} (1 - D_4) C_{11} \\ 1 - \frac{D_2 + D_1}{2} C_{12} \\ 1 - \frac{D_2 + D_3}{2} C_{13} \\ 1 - \frac{D_2 + D_3}{2} C_{13} \\ 1 - \frac{D_3 + D_3}{2} C_{13} \end{bmatrix} \\
& \begin{bmatrix} (1 - D_4) C_{22} \\ (1 - D_2) C_{22} \\ (1 - D_3) C_{23} \\ (1 - D_3) C_{23} \\ (1 - D_2) C_{23} \end{bmatrix} \quad \text{sym} \\
& \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix}
\end{align*}
\]

(13)

| Mode of failure | \( D_1 \) | \( D_2 \) | \( D_3 \) | \( D_4 \) | \( D_5 \) | \( D_6 \) |
|----------------|--------|--------|--------|--------|--------|--------|
| Yarns          | \( H_1 \) | 0.9    | 0.9    | 0.9    | 0.9    | 0.9    |
| \( H_2 \)      | 0.7    | 0.7    | 0.2    | 0.7    | 0.7    | 0.7    |
| Matrix         | 0.8    | 0.8    | 0.8    | 0.8    | 0.8    | 0.8    |

In this paper, the damage criterion and the degradation scheme of material properties are applied into the constitutive relationship of materials by the user-defined extension program APDL command in ANSYS. The damage of each component material element is judged by different damage criteria. The damage is divided into two modes: the axial damage of tows (\( H_1 \)) and the transverse damage of tows (\( H_2 \)). According to different modes, the corresponding material properties are degraded. The progressive damage process analysis diagram of composite materials is shown in figure 6.
5. Result and discussion
As is known, there are many similarities with the typical tensile curves of 1D and 2D composites. The curve has obvious segmentation feature. The first stage is a linear elastic stage with recoverable deformation after unloading, which corresponds to a definite critical stress for damage. The second section of the 3D test curve shows pseudo-linear behavior, and there is no obvious damage generation and expansion stage. The different damage and failure mechanisms of three-dimensional fiber reinforced ceramic matrix composites and low-dimensional corresponding materials are presented. The finite element software ANSYS is used to apply radial (X-direction) load on the tow scale model, which is shown in figure 2. The stress-strain curve of the model under the damage criterion is shown in figure 7. From figure 7, it can be seen that the trend of the simulation curve is basically the same as the test curve. The predicted value of the tensile strength is 251.4 MPa, and the ultimate tensile strain is 0.559%, which is in good agreement with the experimental value, as shown in table 5.
Figure 7. Tensile stress-strain curve of C/SiC composites.

Table 5 Theoretical and experimental results

|                  | Theoretical value | Experimental value[17] |
|------------------|-------------------|------------------------|
| Stress/(MPa)     | 251.4             | 251.3                  |
| Strain/(‰)      | 5.59              | 5.48                   |

It can be seen from the numerical simulation curve that when the stress is small, no damage occurs in the tow scale model, and the stress-strain curve is linear. As the load continues to increase, the damage of tows and SiC matrix (tows mainly produce $H_2$ damage mode) begin to occur, and the curve exhibits nonlinear characteristic. As the load continues to increase, and the tensile load is assumed by carbon fibers due to the saturation of matrix cracks. At this time, the material performance is relatively stable, and the stress-strain curve is linear. When the load increases to a certain extent, damage mode $H_1$ occurs in the tows, which will ultimately lead to the overall damage of the material. Figure 8 shows the tows stress distribution cloud diagram under the tensile load of the model of RVE.

Figure 8. Distribution of stress in the yarns and surface matrix elements damage expansion. (a) $\varepsilon_e = 0.03\%$ (b) $\varepsilon_e = 0.19\%$ (c) $\varepsilon_e = 0.39\%$ (d) $\varepsilon_e = 0.56\%$ composites.

6. Conclusions
In this paper, a micromechanical model is developed to predict the elastic and strength properties of plain woven SiC/SiC composite. The framework of the approach consists of the RVE modeling on fibre
and tow scales, and a two scale computation scheme based on the finite element analysis of RVE. The findings from the experiment and numerical predictions are summarized as follows:

1. Based on the real structure of three-dimensional braided C/SiC composites fabricated by 3D four-step braiding process, a multiscale microstructural model was established, including carbon fiber/PyC interphase/SiC matrix scale and tow/SiC matrix/SiC coating scale.

2. The energy method is used to predict the elastic constants of each component of 3D braided C/SiC composites at multiscale. Based on the theory of periodic boundary conditions and Tsai-Wu failure criterion with failure modes and maximum stress criterion, the strength of the fibre scale model in all directions and the axial tensile strength of tow scale model are predicted. The progressive damage process of 3D braided C/SiC composites was analyzed. The uniaxial tensile stress-strain behavior was simulated. The simulated curves were in good agreement with the experimental ones. The predicted results were close to the experimental results. The effective prediction of the strength of 3D braided C/SiC composites was realized.

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