

MODELING OF 3-D WOVEN CERAMIC MATRIX COMPOSITES

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ABSTRACT

Three different approaches are being pursued at the NASA Glenn Research Center to predict the thermostructural behavior of three-dimensional woven ceramic matrix composites. These are: a micromechanics-based approach using W-CEMCAN (Woven Ceramic Matrix Composite Analyzer), a laminate analogy method and a structural frame approach (based on the finite element method). All three techniques are applied to predict the thermomechanical properties of a three-dimensional woven angle interlock C/SiC composite. The properties are predicted for room temperature and 1100 °C and the predicted properties are compared to measurements. General observations regarding the three approaches for three-dimensional composite modeling are discussed.

KEYWORDS: Ceramic Matrix Composites, Laminate Analogy, Binary Models, Structural Frame Model, Angle Interlock, 3-D Woven Composites

1. BACKGROUND/INTRODUCTION

Ceramic matrix composites (CMC) are emerging materials with high potential payoffs in many aerospace applications. In fact, the development of CMC technology is considered by many as essential to the realization of the next generation reusable launch system. The low density of CMCs and their ability to maintain strength and stiffness at high temperatures are the primary advantages of CMCs over the more conventional launch vehicle and propulsion system materials. The benefits associated with utilizing CMCs will be realized largely by increasing the engine operating temperature, raising temperature safety margins, avoiding the need for cooling, and possibly improved damping capacity, while reducing the launch vehicle weight. No other

material system can accomplish all of these things. However, CMC's suffer from high manufacturing costs and insufficient characterization. Designers do not have an available database with design allowables to have the required confidence in the structures made of CMCs. Credible structural life and performance predictions depend upon understanding composite degradation mechanisms and stress distributions in various constituents. References such as the MIL-handbook that deal with CMCs are in the preliminary stages of development and by their nature represent a work in progress as the state of the art evolves.

Before CMCs find extensive use in space applications, their reliability as hot structures sustaining harsh service environments must be well established. This involves extensive testing and characterization of the materials as well as the development of predictive design/analysis tools. Material characterization efforts based solely on testing are impractical for the time and costs involved. Analytical predictive tools are therefore necessary to bring down the costs and reduce the design cycle time. A synergistic combination of both is therefore desirable for achieving success using the advanced CMC technology. The present paper addresses the latter, namely the development of accurate mathematical models that predict the thermostructural behavior over wide temperature ranges. The primary focus is on modeling a 3-D woven carbon silicon carbide (C/SiC) composite. Herein, three different approaches are applied to model the material. Two of the approaches have their foundations in the familiar micromechanics-based approaches [1]. The third one is based on a structural frame model and resembles closely the binary models [2-3]. Predictions of the CMC properties at room as well as high temperatures are the primary objective of these models. The predictions are compared with the limited available experimental data. In addition, conclusions regarding the effectiveness and accuracy of the various models are drawn based upon the results.

2. APPROACHES

The primary focus of the present study is on the development of methodologies for predicting the properties of 3-D woven angle interlock ceramic matrix composites. As mentioned above, three different modeling approaches are applied to model the 3-D woven composite namely, 1) the structural frame model approach, 2) a micromechanics-based approach and 3) a laminate analogy model-based approach. In the structural frame model approach, the CMC medium is replaced by a structural framework of axial/bending elements and springs. The structural frame is then solved using the finite element technique. In this sense, it is analogous to the 'binary models' [2,3]. The second and the third approaches both have their foundations in micromechanics. In the micromechanics-based approach, a representative volume element capturing all the local details regarding fiber architecture, interface details, fiber and matrix constituents within the tow as well as between the tows is utilized. A mechanics of the materials approach is then applied to arrive at effective properties. The overall properties of the laminate are then obtained by successive application of classical lamination theory. In the laminate analogy modeling [4], the representative volume element is modeled as a superposition of several sub-laminates that capture the fiber architectural details. The properties of each lamina are determined using a conventional micromechanics approach similar to the one used in the previous approach. The superposition of the individual sub-laminates is achieved using classical lamination theory.

2.1 Structural frame model: The fiber architectural details of a three dimensional (3-D) angle interlock C/SiC composite are shown in Figure 1. The weave consists of warp tows and pick tows. Warp tows are woven continuously in an up-and-down pattern through the arrangement of pick tows. The pick tows, which occupy the spaces between the warp weavers, provide the reinforcement in the y-direction, perpendicular to the plane of the warp weavers. The weave uses a pattern of nine warp weavers. This nine-warp tow pattern is repeated, in the y-direction, every “L” inches.

The motivation for representing the C/SiC composite as a structural frame is provided by a close examination of the microstructure. In C/SiC composites, the significant difference in the thermal expansion behavior of the carbon fibers and the SiC matrix, coupled with the temperature excursions during processing, result in high tensile stresses and a highly cracked matrix. In most cases, large void volumes exist between adjacent tows [5]. The microstructure resembles a lattice structure rather than a homogeneous continuum. Cox, et al. [2, 3] developed a model for polymer matrix composites (PMCs) using a combination of axial elements and solid “effective medium” elements. This approach, which they referred to as a Binary Model since it employs two types of elements, is akin to a Netting Analysis technique [1]. The axial elements represent the axial stiffness of individual tows whereas the solid “effective medium” elements are used to represent the stiffness contributions of all other aspects of the composite microstructure, such as inter-tow matrix, voids, and transverse tow properties. The Binary Model does not explicitly account for the effect of the bending and torsion stiffness of the tows on the material response. This effect may be significant for infiltrated C/SiC tows, particularly in the material response to shear stress. Along the same vein as the Binary Model, the Structural Frame Model approach treats the woven composite material as a structure; however, it attempts to eliminate the dependence on the “effective medium element.” In the Structural Frame Model approach, the woven C/SiC material is represented by an assemblage of structural frame elements. These frame elements possess axial, bending and torsion stiffness. The assemblage of elements simulates the internal structure of the woven fiber architecture, as each frame element represents a segment of either a warp or pick (fill) tow.

The details of the structural frame model that was used to simulate the 3-D angle interlock C/SiC composite response are shown in Fig. 2. The model consists of five frames joined together by lateral (y direction) elements. These frames lie parallel to the xz-plane. They effectively represent the arrangement of warp weavers. Each frame is constructed of 162 elements and 95 nodes. The nodal locations correspond to the location in the fiber preform where warp weavers cross over each other (Fig. 1). The lateral elements, which represent the pick tows, are also connected to the frames at the crossover nodes. In order to capture the stiffness provided to the warp weaver by the pick tows, spring elements were added to the model (Fig. 3). The stiffness of the spring elements was estimated based on the transverse stiffness of the pick tows.

The analysis of the structural frame was performed by the ABAQUS Finite Element Program [6]. Six analysis solutions were performed to obtain the Young’s moduli, Poisson’s ratios and the shear moduli in the three principal material directions. Displacement boundary conditions are applied to the structural frame and average stresses in the material are determined from the resulting nodal forces. The elastic moduli are calculated from the applied strains and the calculated average stresses. Poisson’s ratios are determined as the ratio of the off-axis strains to

the applied strain. The boundary conditions which were applied for each analysis solution are shown in Table 1.

Photomicrographs of 3-D angle interlock composite samples reveal that the warp tow cross-section is nearly rectangular, so the cross-sectional area and the moments of inertia about the tow 1-1 and 2-2 axes for the warp tows are estimated by $A = bh$, $I_{11} = bh^3/12$, and $I_{22} = b^3h/12$, respectively. The fill tow cross-section appears elliptic, so the cross-sectional area and the moments of inertia for the fill tows are estimated by $A = \pi ab$, $I_{11} = \pi ab^3/4$, and $I_{22} = \pi a^3b/4$.

The longitudinal modulus of elasticity for the tows E_L is estimated using the rule of mixtures based on the volume fraction of carbon fibers in the tow. That is

$$E_L = v_f E_L^f + (1 - v_f) E^m \quad (1)$$

where v_f is the volume fraction of fibers in the tow, E_L^f is the fiber longitudinal modulus and E^m is the matrix Young's modulus. The stiffness contributed from the inter-tow matrix is neglected. The value for the fiber longitudinal modulus that was used in the analysis is listed in Table 2. It is assumed that the fiber stiffness is constant over the temperature range considered in this study. As the SiC matrix is cracked due to processing residual stresses, the matrix in-situ stiffness is dependent upon the temperature and the composite strain state. In this study, various values for the matrix modulus were assumed depending on the temperature and strain state being simulated.

2.2 Micromechanics-based approach: NASA Glenn Research Center has been actively involved in the development of micromechanics-based approaches for predicting the thermal and mechanical properties of both 2-D and 3-D woven CMC's. A novel micromechanics-based technique to predict the thermal and mechanical properties of 2-D advanced woven ceramic matrix composites was developed and programmed into a computer code called W-CEMCAN (Woven Ceramic Matrix Composite Analyzer). This technique was used previously [7] to characterize the properties of a 0/90 plain-weave C/SiC (T-300 carbon fibers in a chemical vapor infiltrated silicon carbide matrix) composite. The available measured composite properties of a 0/90 plain weave C/SiC composite were used to establish a calibrated temperature-dependent constituent property database. Once established, the constituent material property database is utilized to predict a full set of three-dimensional composite properties needed in the design and analysis of structural components. These analyses also help the material development effort in optimizing key composite properties for specific applications.

In the present study, the approach mentioned above is modified to simulate the composite behavior with three-dimensional fiber architectures. In this work, a three-dimensional angle interlock fiber architecture is evaluated. The approach used is similar to that used for 2-D fiber architectures with modifications to account for the three-dimensional fiber geometry. Figure 1 shows a representative volume element (unit cell) of the 3-D angle interlock architecture under investigation. The unit cell is divided into several slices of equal width w as shown in Figure 4.

The number of slices is a user input parameter. Each slice of width w contains pick fibers at a 90° orientation as well as warp-weavers at $\pm\theta^\circ$ angles. This angle as well as the volume fractions of the pick and warp weavers is calculated from the known geometry. Thus it will be assumed that each slice of width w contains plies at 90° , plies at $\pm\theta^\circ$ (in the X-Z) plane as well as a matrix-rich region with no fibers. It is also assumed that the classical laminate theory is applicable at each section of the model. The slice with width w will then be analyzed as a regular "laminate" consisting of the above-mentioned "plies". In a regular laminate, plies are oriented in the X-Y plane, while the warp-weavers are oriented at $\pm\theta^\circ$ in the X-Z plane. To take into account this orientation, this slice is analyzed twice to get all the properties as explained in Reference [7]. Once the equivalent properties of a particular slice are obtained, these slices are stacked as "plies" in a laminate and the laminate analysis is used again to compute the overall properties of the unit cell.

2.3 Laminate Analogy Models (LAMS): Laminate analogy is a powerful tool that can be utilized to compute the overall homogenized anisotropic properties of any composite. It relies on stiffness averaging principles via judicious use of classical laminate theory. Such modeling techniques have been used in the past by several researchers [4, 8]. To arrive at the effective anisotropic properties of the 3-D angle interlock C/SiC, one can use the traditional micromechanics-based approach combined with laminate analogy models.

Central to the micromechanics-based approaches is the definition/identification of a representative volume element or a unit cell. Figure 5 shows the unit cell that is considered for the current approach. As shown, the unit cell typically consists of three distinct constituents: fiber, matrix and interphase/coating. The three constituents are assumed to have an independent set of properties. The unit cell is further divided into several slices and a typical slice can have three distinct regions namely fiber, matrix and interphase as shown in Figure 5b. Micromechanics for the unit cell yield typically a ply or lamina level properties. The in-house developed CEMCAN (Ceramic Matrix Composite Analyzer) computer code [9] is based on such a model and is utilized for the current effort. References [9-10] give the relevant details regarding lamina level properties and the computer code.

The 3-D angle interlock woven structure is shown in Figure 1. In the laminate analogy modeling, this particular architecture is modeled as a superposition of three laminates. The first laminate consists of pick tows which are modeled as nine $[90]$ degree plies. The second and the third laminates consisting of the warp tows are modeled as five $[\pm\theta]$ plies. It should be noted that the angle is with respect to the thickness axis, Z. Appropriate transformations have to be applied to the ply properties representing the angle interlocks in order to combine them with the $[90]$ plies. Based upon the actual number of pick fiber yarns and the angle interlock yarns, the fiber volume ratios for the $[90]$ and $[\pm\theta]$ are determined.

The steps involved in the laminate analogy model are listed below:

1. By using fiber substructuring and unit cell models the ply/lamina properties are computed. The details are given in references [9-10].

2. The 3-D angle interlock woven CMC system is then modeled as a superposition of three sub-laminates following the laminate analogy. The properties of the individual plies in these laminates are obtained in step 1.
3. By using the laminate analogy and superposition principles the 3-D homogenization is accomplished and the overall properties of the 3-D angle interlock woven CMC system are computed.

In the above the step 1 is already available through CEMCAN computer code [9]. Step 2 requires additional programming and augmentation to the CEMCAN computer code.

Both the micromechanics and the laminate analogy approaches can handle temperature dependent property via a functional relationship that ties the room temperature constituent property to property at any use temperature. The relationship used is the following:

$$\frac{P}{P_0} = \left[\frac{T_f - T}{T_f - T_0} \right]^n \quad (2)$$

where P is the constituent property at temperature T, and P₀ is the reference property at temperature T₀, usually the room-temperature. T_f is the final temperature where the property is nearly zero and “n” is an exponent describing the shape of the curve from reference to the final property. The constants in the relationship above have to be established based on some experimental measurements taken at different temperatures. In the absence of such, or if the relationship is not monotonous, the constituent properties at different temperatures can be given in the form of a table as well. In the present study, measurement of composite properties at several temperatures are planned therefore such relationships as above can be utilized. However, at the time of reporting, these measurements are still not complete.

3 RESULTS/PREDICTIONS OF THREE DIFFERENT APPROACHES

All three material modeling techniques require key information from the experimental investigations as well as properties of the constituents. The constituent level information is essential for the two micromechanics-based approaches as well as for the Structural Frame approach. Typical room temperature constituent properties that are used in the predictions are given in Tables 2, 3 and 4. The fiber tow is made of T300 fibers. The coating properties are typical of a carbon coating. The matrix properties are for bulk CVI SiC. A typical value for CVI SiC matrix bulk modulus is around 420 GPa and thermal conductivity is about 46 W/m-K for a fully dense matrix. Since it is known that the matrix is highly cracked in the as-fabricated condition, for the reasons mentioned before, the in-situ matrix stiffness is expected to be much lower than the value shown in Table 3. The true in-situ matrix stiffness needs to be calibrated from measured composite data and by exercising the material models.

Predictions of the room temperature response properties, such as the shear and Young’s modulus and the Poisson’s ratio, obtained using the three modeling approaches, are listed in Table 5. The predictions were made by assuming a value of 6.9 and 69 GPa for the matrix Young’s modulus. It should be noted that these predictions are intended to simulate the response properties at very low applied stress levels. The measured data (an average of three coupon tests) shown in Table 5 are also the initial values reported in Reference [11]. The warp modulus predictions by all three

approaches are similar. The measured warp modulus is in the middle of the predicted range. In the case of the fill direction modulus (E_f or E_{yy}), the measured value is in the middle of the range predicted by the micromechanics and LAMS approaches. The structural frame model predicted close to the measured value when the lower limit is chosen for the in-situ matrix stiffness. In regard to the through-thickness modulus, the predictions by the micromechanics and LAMS approaches are much higher than that predicted by the structural frame model. The reason is in the structural frame model, no stiffness is contributed to the Z direction by the transverse stiffness of the warp weavers. Also, the structural frame model assumes that the inter tow matrix contributes no stiffness. The measurements for the through-thickness modulus (E_{zz}) are not available. In regard to the in-plane shear modulus (G_{wf} or G_{xy}), the measured value is in the middle of the range predicted by both the micromechanics and the LAMS approaches. The structural frame model predicts much closer to the measured value while using the higher value for the in-situ modulus. The measured Poisson's ratio is almost negligible and is considerably lower than the predictions of the micromechanics and LAMS approaches. Such a low value clearly indicates a lack of coupling between the fill and warp directions which must be the result of excessively cracked matrix. The structural frame model does not have a coupling between fill and warp directions and therefore predicts zero for Poisson's ratio.

Predictions of the response properties at 1100 °C obtained using the three modeling approaches are shown in Table 6. As the temperature increases, the residual stresses are relieved thereby closing the matrix micro cracks. This increases the overall stiffness of the composite by decreasing the in-situ matrix compliance. In order to account for this phenomenon, the estimates of the in-situ matrix modulus are increased. In predicting the 1100 °C composite properties, the values of 138 and 173 GPa were assumed for the matrix Young's modulus. The fiber modulus is assumed to be unchanged at these temperatures in the calculations. The fill direction modulus predictions obtained by all three approaches are similar. The measured value, however, is slightly lower than the lower limits predicted by all three approaches. No measured data was available for the in-plane shear and through-thickness moduli at the time of writing this report. The micromechanics and LAMS predictions are higher than the structural frame predictions for both the in-plane shear and through-thickness moduli.

Thermal property predictions are shown in Table 7. Although, the table only shows the predictions by LAMS, the predictions using micromechanics were essentially identical to the LAMS approach. The predicted thermal expansion coefficients agree well with the measured data for the higher temperatures. However, the room temperature predictions are not in good agreement. The reason for this appears to be due to the negative expansion coefficient of T300 fiber. Also, it was much harder to extract and compute the coefficient of thermal expansion at the starting point of the measured data. The measurements are made for total expansion of the test coupon, starting from room temperature, which makes it difficult to estimate the expansion at room temperature. The prediction of the thermal conductivity appears to be in excellent agreement with measured data for warp and through-the-thickness directions. At the time of writing the predictions according to the structural frame model for the conductivities and the expansion coefficients as well as the measurements for the fill direction conductivities are not available.

4 CONCLUDING REMARKS AND FUTURE DIRECTIONS

The micromechanics and LAMS approaches yielded similar predictions. This is to be expected, since they have a similar micromechanics-based foundation. The structural frame approach predictions are somewhat different from that of the other two. However, it can be concluded that all three methods seem to be viable material modeling techniques for predicting the response properties for 3-D woven angle interlock C/SiC composites.

By exercising the three modeling approaches to simulate the material response, it became evident that the in-situ matrix stiffness in the composite specimens was only a fraction of the stiffness of SiC in its bulk form (420 GPa). The reduction in the matrix stiffness being attributed to matrix cracking as a result of processing stresses. The results of this study highlight the importance of assessing the in-situ matrix stiffness correctly, as its assumed value significantly influences the response property predictions. Future efforts should concentrate on defining the matrix stiffness as a function of temperature and composite strain state.

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TABLES

Table 1. Summary of Boundary Conditions Used for the Structural Frame Analysis Solutions

Analysis Solution	Solution Results Determine	Boundary conditions
1	E_x, ν_{xy} and ν_{xz}	$@x = 0, u_x = 0$ $@x = L, u_x = e_x L$
2	E_y, ν_{yx} and ν_{yz}	$@y = 0, u_y = 0$ $@y = W, u_y = e_y W$
3	E_z, ν_{zx} and ν_{zy}	$@z = 0, u_z = 0$ $@z = h, u_z = e_z h$
4	G_{xz}	$@z = 0, u_x = u_z = 0$ $@z = h, u_x = \gamma_{xz} h$
5	G_{yz}	$@z = 0, u_y = u_z = 0$ $@z = h, u_y = \gamma_{yz} h$
6	G_{xy}	$@y = 0, u_x = u_y = 0$ $@y = W, u_x = \gamma_{xy} W$

Table 2. Fiber Properties

Property	Value
Modulus (11)	231 GPa
Modulus (22)	22.4 GPa
Poisson's Ratio (12)	.3
Poisson's Ratio (23)	.35
Shear Modulus (12)	22.4 GPa
Shear Modulus (23)	22 GPa
CTE 11	-.99 ppm/deg. K
CTE 22	4.5 ppm/deg. K
Conductivity (11)	18.13 w/mK
Conductivity (22)	4.42 w/mK
Density	1.77 Mg/m ³

Table 3. Typical Room Temperature Matrix Properties

Property	Value
Poisson's Ratio	.2
Modulus	420 GPa
Thermal Exp. Coeff.	2.63 ppm/deg. K
Conductivity	45.62 w/mK
Density	3.21 Mg/ m ³

Table 4. Interface Properties

Property	Value
Modulus	.69 GPa
Poisson's Ratio	.17
Thermal Exp. Coeff.	1.8 w/mK
Conductivity	0.02w/mK
Density	2.18 Mg/ m ³

Table 5. Comparison of Material Model Results and Measured Properties at Room Temperature

Property	Predictions						Average Measured Data
	Micro-mechanics		LAMS		Structural Frame		
	$E_m=6.9$ GPa	$E_m=69$ GPa	$E_m=6.9$ GPa	$E_m=69$ GPa	$E_m=6.9$ GPa	$E_m=69$ GPa	
E_w , GPa	47.6	77.3	56.6	73.8	52.2	68.0	66.5
E_f , GPa	29.7	49	29	55.2	39.7	51.8	38.2
E_z , GPa	7.6	25.5	7.5	24.4	4.8	6	-
ν_{wf}	0.06	0.13	0.04	0.09	0.0	0.0	0.03
G_{wf} , GPa	3.8	13.1	3.2	12.4	5.3	7.0	8.1

Table 6. Comparison of Material Model Results and Measured Properties at 1100 °C

Property	Predictions						Average Measured Data
	Micro-mechanics		LAMS		Structural Frame		
	$E_m=138$ GPa	$E_m=173$ GPa	$E_m=138$ GPa	$E_m=173$ GPa	$E_m=138$ GPa	$E_m=173$ GPa	
E_w , GPa	95.8	105	98.7	109	83.8	91.7	103.5
E_f , GPa	65.5	73	62.1	73.8	63.8	69.8	61.3
E_z , GPa	35.8	41	40	46.2	7	-	-
ν_{wf}	.11	.13	0.12	0.12	0	-	-
G_{wf} , GPa	19	22	19	21.6	8.5	-	-

Table 7. Thermal Properties of 3-D C/SiC Composite

Property	T = 21°C		T = 538°C		T = 1100°C	
	LAMS	Exp.	LAMS	Exp.	LAMS	Exp.
$\alpha_w, 10^{-6}/^{\circ}\text{C}$	0.9	~0	1.2	0.9	2.2	2.0
$\alpha_F, 10^{-6}/^{\circ}\text{C}$	1.6	~0	2.2	1.8	3.2	2.7
$\alpha_z, 10^{-6}/^{\circ}\text{C}$	3.1	1.8	3.8	3.6	5.4	5.4
$K_w, \text{W/mK}$	19.7	20.8	18.5	21.5	17.0	20*
$K_F, \text{W/mK}$	11.4	-	10.8	-	9.8	-
$K_z, \text{W/mK}$	5.2	4.3	4.8	4.3	4.2	3.6*

* extrapolated

(LAMS and Micromechanics predictions are nearly identical.)

FIGURES

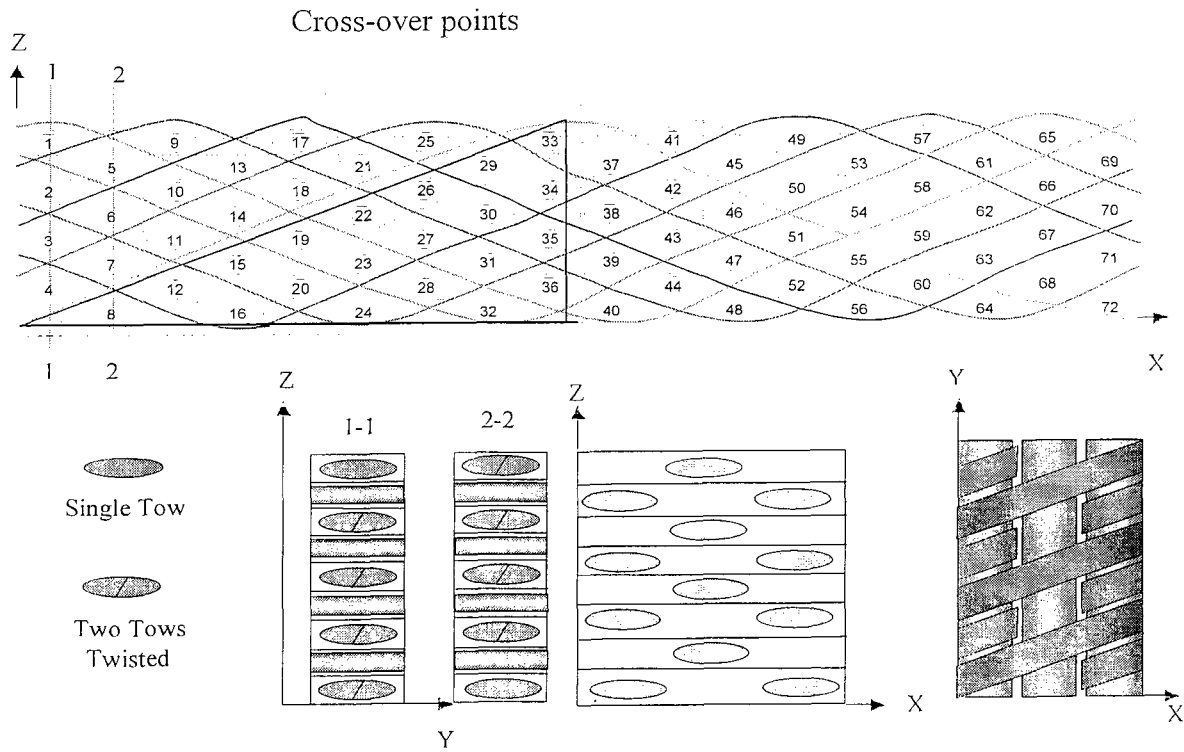


Figure 1. Geometric and modeling details of the 3-D Angle Interlock woven CMC composite system.

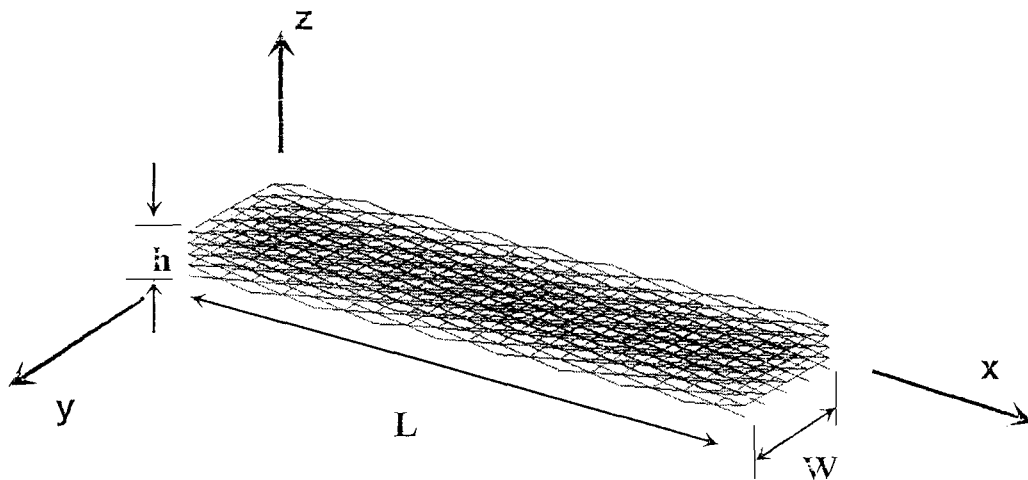


Figure 2. Sketch of frame used to simulate 3-D Angle Interlock Composite

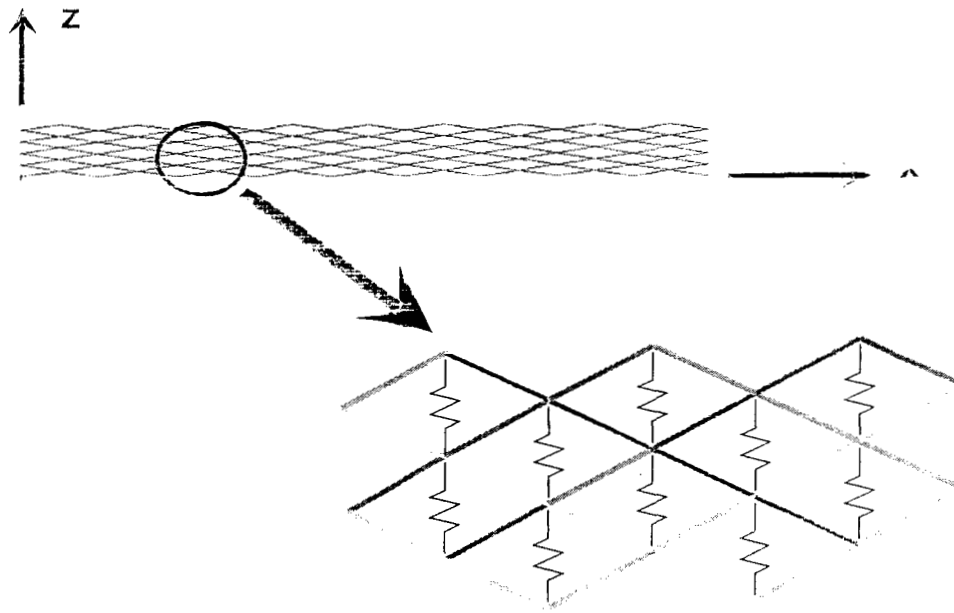


Figure 3. Sketch showing the position of spring elements in the finite element model.

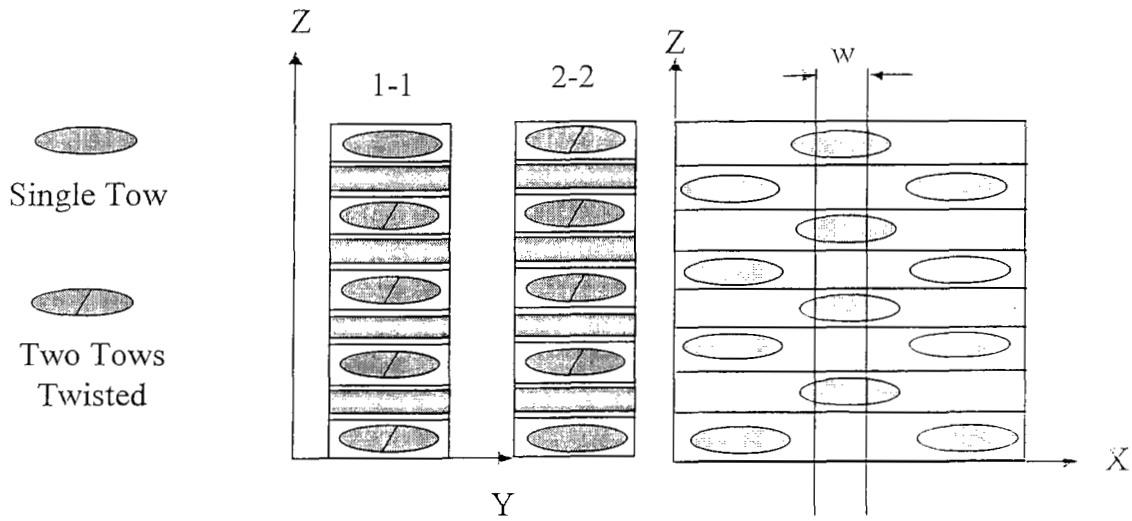


Figure 4. Details of slicing of the representative volume element of 3-D Angle Interlock weave.

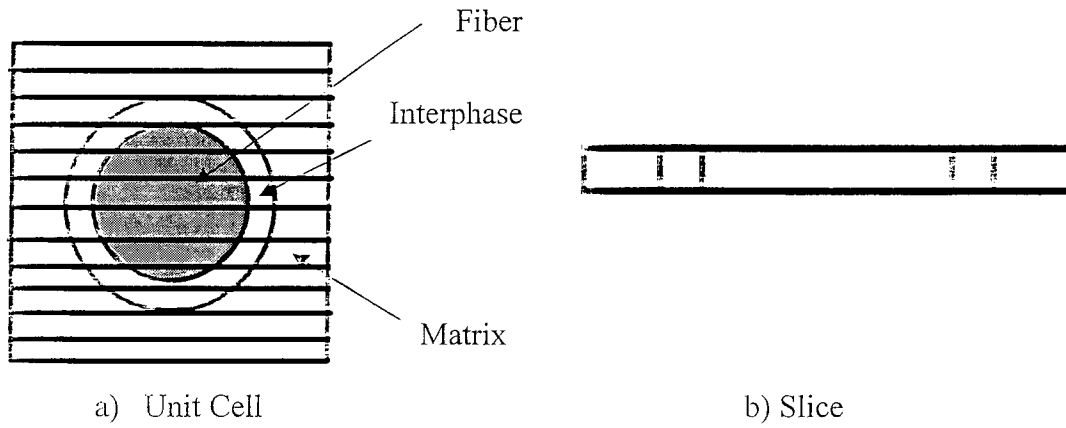


Figure 5. Representative volume element (RVE) for CMC's.

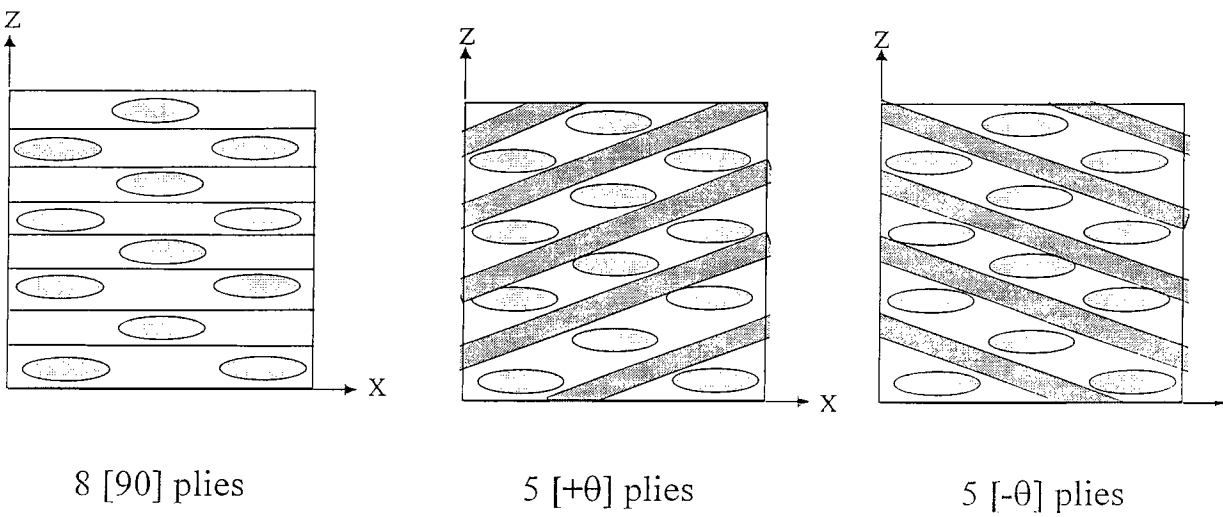


Figure 6. Superposition details of [90], and $[\pm \theta]$ plies to approximate the 3-D Angle Interlock woven composite.