Stochastic Multiscale Modeling and Statistical Characterization of
Complex Polymer Matrix Composites

by
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ABSTRACT

There are many applications for polymer matrix composite materials in a variety of different industries, but designing and modeling with these materials remains a challenge due to the intricate architecture and damage modes. Multiscale modeling techniques of composite structures subjected to complex loadings are needed in order to address the scale-dependent behavior and failure. The rate dependency and nonlinearity of polymer matrix composite materials further complicates the modeling. Additionally, variability in the material constituents plays an important role in the material behavior and damage. The systematic consideration of uncertainties is as important as having the appropriate structural model, especially during model validation where the total error between physical observation and model prediction must be characterized. It is necessary to quantify the effects of uncertainties at every length scale in order to fully understand their impact on the structural response. Material variability may include variations in fiber volume fraction, fiber dimensions, fiber waviness, pure resin pockets, and void distributions. Therefore, a stochastic modeling framework with scale dependent constitutive laws and an appropriate failure theory is required to simulate the behavior and failure of polymer matrix composite structures subjected to complex loadings. Additionally, the variations in environmental conditions for aerospace applications and the effect of these conditions on the polymer matrix composite material need to be considered. The research presented in this dissertation provides the framework for stochastic multiscale modeling of composites and the characterization data needed to determine the effect of different environmental conditions on the material properties. The developed models extend sectional micromechanics techniques by incorporating 3D progressive damage theories and
multiscale failure criteria. The mechanical testing of composites under various environmental conditions demonstrates the degrading effect these conditions have on the elastic and failure properties of the material. The methodologies presented in this research represent substantial progress toward understanding the failure and effect of variability for complex polymer matrix composites.
This dissertation is dedicated to my wife, daughter, and son,

as well as my parents and my wife’s parents,

for their love, encouragement, support, and patience.

Thanks to all of you, this work is possible.
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1. INTRODUCTION

1.1. Motivation

Polymer matrix composite (PMC) materials are increasingly being used in airframe and engine applications. However, damage initiation and failure mechanisms in composites are still not fully understood and are an ongoing area of research. A multiscale modeling framework with scale-dependent constitutive laws and an appropriate failure theory is required to capture the behavior and failure of composite structures. For the failure of engine containment systems, such as a fan blade separating from the rotor during operation, the system’s ability to prevent impact failure and decrease the severity of an impact event on the surrounding components is essential. The rate dependency and nonlinearity of PMC materials further increases the complexity of the models required to simulate an impact event. Additionally, variability in the material constituents plays an important role in the material’s behavior and damage. The systematic consideration of uncertainties is as important as having an appropriate structural model, especially during model validation where the total error between physical observation and model prediction must be characterized. It is necessary, therefore, to quantify the effects of uncertainties at every length scale, in order to fully understand their impact on the structural response. Material variability can include variations in fiber volume fraction ($V_f$), fiber dimensions, fiber waviness, pure resin pockets, and void distributions. With this in mind, a stochastic modeling framework with scale-dependent constitutive laws and an appropriate failure theory is required to simulate the behavior and failure of PMC structures. The multiscale model must have the ability to account for variability, strain rate effects, through-thickness
shear stresses, and environmental conditions, so that it can reliably determine the material’s applicability for aerospace structures and components.

1.2. Composite Micromechanics

Various micromechanical models have been developed to simulate the behavior and effective properties of PMCs. Using a mechanics of materials approach (Hill, 1964; Shaffer, 1964), the composite model is discretized into two rectangular phases where the phases are either in parallel (Voigt, 1889) with equal uniform strain assumptions, or the phases are in series (Reuss, 1929) with equal uniform stress assumptions. However, the mechanics of materials approach is inaccurate when calculating the effective transverse and shear properties. The concentric cylinder assemblage model that Hashin and Rosen (1964) developed applies a similar separation into two cylindrical phases for the fiber and matrix. The self-consistent method is able to predict the effective moduli of a composite by assuming a single particle in an effective medium, which reduces to the solution of a single inclusion in an infinite effective medium (Eshelby, 1957). The Mori-Tanaka model (Mori & Tanaka, 1973) assumes the average strain computed for the matrix correlates to the average strain of a fiber or particle. By discretizing the composite unit cell into three subcells, Sun and Chen (1991) were able to develop a 2D elastic-plastic model that was later extended to three dimensions by Robertson and Mall (1993). Whitney (1993) proposed a more precise elastic micromechanics model where the unit cell was divided into an arbitrary number of rectangular, horizontal slices. Mital et al. (1995) used a slicing approach to compute the effective elastic constants and microstresses (fiber and matrix stresses) in ceramic matrix composites, and a mechanics of materials approach was used
to compute the effective elastic constants and microstresses in each slice of a unit cell. Laminate theory was then applied to obtain the effective elastic constants not only for the unit cell, but also for the effective stresses in each slice. The slicing approach was extended to include material nonlinearity and strain rate dependency in a deformation analysis of PMCs, and then used to investigate the response of thin laminated plates subjected to in-plane loading (Goldberg, 2000, 2001; Goldberg, Roberts, & Gilat, 2004, 2005). This slice micromechanical model was further modified to incorporate out-of-plane, transverse shear effects to simulate the transient and impact responses of composite shells (Zhu, 2006; Zhu, Chattopadhyay, & Goldberg, 2006b; Zhu, Kim, Chattopadhyay, & Goldberg, 2005). The slice model was next extended to a 3D sectional micromechanics model (Zhu, 2006; Zhu, Chattopadhyay, & Goldberg, 2006a, 2008). The sectional micromechanics model applied a decoupling concept to the fiber/matrix unit cell that captured the full 3D stress and strain components in a computationally efficient manner and preserved the transverse isotropy of the material. The method of cells (MOC) theory developed by Aboudi (1981, 1989, 2013) discretizes a unidirectional fiber-reinforced composite unit cell into four rectangular subvolumes, called subcells, where one subcell represents the fiber and the remaining three subcells indicate the matrix. The displacement conditions in the MOC theory are assumed to be linear and continuous between the subcells. Paley and Aboudi (1992) expanded the MOC approach into a generalized method of cells (GMC) for unidirectional composites, which improved the discretization technique by better capturing the physical shape of the fiber in the unit cell. Pindera and Bednarcyk (2000; 1999) reformulated the GMC using simplified uniform stress and strain assumptions, resulting in improved computational efficiency of the theory. A major limitation of the aforementioned micromechanical
models is that only the homogenized local stress and strain fields can be computed because the exact shear coupling between constituents is not accurately captured. In determining the effective material properties, the effect of shear coupling is minimal; however, shear coupling becomes important when investigating fiber/matrix interface concentrations and local damage and failure of the constituents. For this reason, Aboudi et al. (2001, 2002, 2003) developed the high fidelity generalized method of cells (HFGMC) method, which advances the previous GMC method by integrating a second-order displacement field that is capable of accounting for shear coupling between subcells.

1.2.1. Viscoplastic Theories for Polymer Matrix Composites

A key component for micromechanics based models of PMCs is capturing the essential nonlinear, rate-dependent behavior using viscoplastic theories. Sun and Chen (1989) developed a single parameter plasticity model consisting of a quadratic yield function, associated flow rule, and plastic potential to capture the nonlinear behavior of composites. Another study, by Tsai and Sun (2002), determined the optimal specimen geometry needed to characterize the state variables for a single parameter plasticity model with strain rate effects. Thiruppukuzhi and Sun (2001) developed a two-parameter and three-parameter overstress viscoplastic theory with a rate-dependent failure criterion. The strain rate-dependent behavior of composites has also been modeled using a quadratic stress function in an overstress viscoplastic theory (Gates & Sun, 1991), a constant rate power and 3D viscoplastic law (Weeks & Sun, 1998), and an overstress viscoplastic model that included multiaxial effects (Eisenberg & Yen, 1981). Many viscoplastic theories were adapted from classical plasticity and viscoplasticity theories of metals where hydrostatic
stresses have minimal effect. However, the effect of hydrostatic stresses for polymers has been shown to be significant (Spitzig & Richmond, 1979; Ward & Sweeney, 2012), and several studies have analyzed the nonlinear behavior of polymers by incorporating hydrostatic terms in viscoplastic theories (Chang & Pan, 1997; Hsu, Vogler, & Kyriakides, 1999; F. Z. Li & Pan, 1990). Goldberg et al. (2003) integrated hydrostatic terms in a viscoplastic theory to account for the high strain rate deformation of polymers. They later extended the model by applying an associative flow rule to the viscoplastic theory in order to resolve inaccuracies in the predictions for multiaxial stress states of the polymer (Goldberg et al., 2005).

1.2.2. Interface/Interphase Considerations

Although recent research has shown that the interphase plays a critical role in the performance of PMCs, accurate modeling of the interphase is challenging due to the small scale of this region. Reifsnider (1994) conducted a parametric study using the tensile strength of the interphase as a variable within micromechanical models to investigate the effect on the strength and life of unidirectional composites. Asp et al. (1996) assumed symmetrical and periodic conditions in a finite element analysis (FEA) to model a quarter of the fiber in polymer matrix and considered the effects of interphase thickness on the response through a parametric study of various assumed elastic interphase moduli. Souza et al. (2008) developed a multiscale FEA model by incorporating viscoelasticity in the micromechanics and a cohesive zone law for the interphase to determine the effect of damage under impact loading. FEA has also been used to model representative volume elements (RVEs) with multiple fibers where the interphase was represented by bilinear
cohesive laws (Wang, Zhang, Wang, Zhou, & Sun, 2011; B. Zhang, Yang, Sun, & Tang, 2010). Similar types of interfacial laws have been applied to subcell boundary conditions in the MOC (Aboudi, 1987; Aboudi, 1988) and GMC (Aboudi, 1993; Goldberg and Arnold, 2000; Bednarcyk and Arnold, 2002) theories. Although these studies have applied interfacial laws to account for the fiber/matrix interaction, these microscale interfacial laws are based on large-scale coupon testing or deductions and assumptions from parametric studies. Due to the current limitations in experimental techniques, it is difficult to measure and observe the behavior and failure of the interphase at the atomic/molecular scale, but various test methods have been established using single fiber specimens to measure the fiber/polymer interphase strength (Zhandarov & Mäder, 2005). One such method, called the Broutman test, was originally designed to measure the interphase transverse tensile strength for glass fiber-reinforced PMCs (Broutman, 1969), but it has also been extended to carbon fiber-reinforced PMCs (Ageorges, Friedrich, & Ye, 1999). However, this method calculates the transverse tensile strength using the difference in Poisson ratios between the fiber and polymer matrix under a compressive loading condition, and the transverse modulus cannot be measured from this test. While these experimental studies are capable of estimating interphase properties, the techniques are based on an indirect calculation of the properties and thus cannot capture the full range of material properties required to incorporate the interphase within a multiscale analysis.

In order to overcome the nanoscale experimental limitations, a significant amount of modeling research has been reported to study the molecular scale properties of composites; this includes ab-initio quantum chemistry, density functional theory, and molecular dynamics (MD) methods. For these molecular modeling methods, carbon fiber is often
approximated as graphene or carbon nanotube (CNT) in order to reduce the number of atoms needed to fully represent the fiber. In a study by Hadden et al. (2015), MD-generated properties of graphene nanoplatelets in epoxy were integrated within a multiscale model using GMC micromechanics. Jiang et al. (2013; 2007) modeled the macroscopic behavior of CNT-reinforced nanocomposites using a form of rule of mixtures. In their work, the interphase between the polymer matrix and a CNT is modeled as a wavy surface, and a cohesive stress law is formulated based on the Lennard-Jones potential. Zhang et al. (2010) estimated the mechanical properties of a carbon fiber/polymer interphase by representing the fiber as multiple layers of graphene and constructing a cohesive law using the van der Waals interactions between the constituents. A vast majority of these molecular interphase models are formulated using only the Lennard-Jones potential, which does not account for mechanical entanglements or covalent bond breakage within the constituents. Additionally, graphene and CNTs possess crystalline structures, whereas carbon fiber is semi-crystalline with chains of carbon atoms randomly folded and/or interlocked together (Edwards, Menendez, & Marsh, 2013; Guigon & Oberlin, 1986; Johnson, 1987). Due to the complexity of the carbon fiber, CNT and graphene molecular models cannot be directly applied to simulate the carbon fiber or the fiber interphase.

1.2.3. Damage Mechanics and Failure

The determination of damage and failure is a significant part in modeling the composite response and poses many challenges due to the complexity and plethora of scale-dependent failure and damage modes in such materials. As with many aspects of composites modeling, the failure theories are adaptations of theories developed for
isotropic materials. Hill (1948) modified failure criteria to create a theory for anisotropic metals, and Azzi and Tsai (1965) adjusted the theory for composites. Tsai (1968) also introduced quadratic failure theories to capture the interactions between different stress components. For composites, the strengths in tension and compression directions can differ significantly, and this trait of the material was considered by Tsai and Wu (1971).

The Hashin-Rotem theory (Hashin & Rotem, 1973; Rotem & Hashin, 1976) separated composite failure into individual fiber and matrix failure modes using a quadratic expression. Hashin (1980) later modified the theory to add the difference between tension and compression strengths. A large step towards assessing and modifying these failure theories for composites was the initiation of the World Wide Failure Exercise (WWFE). The WWFE began in 1996 and consisted of a comprehensive experiment and constituent property database for PMCs (Hinton & Soden, 1998; Soden, Hinton, & Kaddour, 1998b, 2002). The database was comprised of a broad range of parameters, including different constituent properties, laminate sequences, and loading conditions. The participants were provided the same material data, and the results from their PMC failure theory predictions were compared with the experimental data. At the end of the WWFE, in 2004, assessments had been made for 19 different failure prediction approaches, and the leading theories were recommended for design purposes (Soden, Hinton, and Kaddour, 1998a; Hinton, Kaddour, and Soden, 2002; Hinton, Kaddour, and Soden, 2004; Kaddour, Hinton, and Soden, 2004; Soden, Kaddour, and Hinton, 2004). The benefits resulting from the WWFE effort were the improvement of many failure theories and the provision of organized publications in which design engineers could access and compare. Despite the success of the WWFE, the exercise was focused on in-plane, biaxial loadings and did not consider the 3D triaxial state
of the material. In response to this deficiency, a second World Wide Failure Exercise (WWFE-II) was initiated in 2007, and the test cases included the failure of neat polymer resin under triaxial loading as well as the triaxial behavior of unidirectional and multidirectional laminates (Hinton & Kaddour, 2012). The study ended in 2012 with 12 groups participating using different methods, and the models were benchmarked (Kaddour & Hinton, 2012a, 2012b, 2013).

The WWFE-II achieved similar accuracy and advances to that shown in the results of the WWFE-I and recognized that the effect due to small-scale needed to be studied; therefore, a third World Wide Failure Exercise (WWFE-III) began. The WWFE-III is currently ongoing, aiming to integrate continuum damage mechanics with the developed and modified failure theories to account for the progression of matrix cracking and delamination (Kaddour, Hinton, Smith, & Li, 2013). Continuum damage mechanics was created as a method for capturing the nonlinear behavior of composites with one of the first damage theories developed by Kachanov (1958, 2013). The basic concept of continuum damage mechanics is introducing damage variables and evolution theories to represent the physical damage initiation and propagation. This is achieved by using the damage parameters to degrade the components of the stiffness tensor by progressively increasing the variables using damage evolution functions that can be formulated with various methods (Allen, Harris, and Groves, 1987a; Allen, Harris, and Groves, 1987b; Paas, Schreurs, and Brekelmans, 1993; Talreja, 1994; Matzenmiller, Lubliner, and Taylor, 1995; Bednarcyk, Aboudi, and Arnold, 2010). Several participants from the first two exercises started developing damage theories for composites before the start of the WWFE-III (McCartney, 1992, 1998; Talreja, 1985, 1994), and a few even employed damage theories
with complex failure criteria (Pinho, Davila, Camanho, Iannucci, & Robinson, 2005; Puck & Schürmann, 1998, 2002). The studies that have been published to date, using the WWFE-III parameters, feature a broad range of techniques including multiscale, energy-based, and cohesive zone models, to name only a few (Carrere, Laurin, and Maire, 2012; Soutis, 2012; Daghia and Ladeveze, 2013; Chamis et al., 2013; Kashtalyan and Soutis, 2013; McCartney, 2013a; McCartney, 2013b; Pinho, Vyas, and Robinson, 2013; Singh and Talreja, 2013).

1.3. Multiscale Composite Modeling

The accurate multiscale modeling of composites can reduce the time and expense required for extensive experimentation. A key factor in modeling composite behavior for aerospace applications, and specifically fan containment systems, is accurately modeling impact loadings and the transient response in the components due to impact. Multiscale models allow the scaling of information between different length scales using homogenization and localization techniques. Several techniques strictly use FEA as the modeling approach, where a small-length scale is simulated and information is transferred to an FEA integration point of a large-scale model (Feyel, 1999; Feyel & Chaboche, 2000). However, running simulations using this technique can be computationally expensive. Micromechanical methods such as asymptotic field expansion separate the fields of the large-scale model into small-scale ones (Fish, Shek, Pandheeradi, & Shephard, 1997; Fish, Yu, & Shek, 1999; Suquet, 1987). The bridging of these scales is performed using the homogenization functions obtainable from a variety of techniques (Fish et al., 1997; Fish & Yu, 2001; Oskay & Fish, 2007). The Voronoi cell method (Ghosh, 2011; Ghosh, Lee,
& Moorthy, 1995; Ghosh & Liu, 1995; Ghosh & Moorthy, 1995; Ghosh & Mukhopadhyay, 1991) analyzes the microscale by explicitly accounting for the composite microstructure using tessellations of polygons containing a single fiber or particle within an FEA formulation. Ghosh et al. (2001) used the approach to develop a multiscale analysis that uses random microstructures to analyze composite failure. The GMC micromechanics technique has been implemented with FEA where each integration point is represented using a single GMC simulation (Wilt, 1995). The Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) (Bednarcyk & Arnold, 2002b, 2007) uses the GMC and HFGMC micromechanics techniques, as well as classical laminate theory (Herakovich, 1998; Jones, 1975), to conduct multiscale analyses of composites. Liu et al. (2011a; 2011b; 2011c) developed a Multiscale Generalized Method of Cells (MSGMC) framework, which performed through-thickness homogenization, introducing normal/shear coupling, to study the material behavior and failure of composites with complex architectures. Chamis (2004) presented a stochastic multiscale framework that used fast probability integration to incorporate uncertainty in the material properties.

1.4. Triaxial Braid Composite Models

Modeling triaxial braided PMCs is a difficult task, due to the material’s nonlinearity and architectural variability. Naik et al. (1995; 1994) used a volume averaging, homogenization technique with iso-strain assumptions within the triaxial repeating unit cell (RUC) to calculate the material properties. Quek et al. (2003) implemented concentric cylinder micromechanics within the RUC and modeled the tow undulations as waveforms. Song et al. (2007) modeled a single RUC in compression using finite element-based
micromechanics. Cheng and Binienda (2008) used a through-thickness braiding approach of the RUC by employing various stacking sequences to model the different subcells of the RUC. Littell et al. (2008a; 2008b) also used this type of braiding approach for the RUC, but incorporated an idealized tow shift rule to account for the overlapping of the axial tows through the thickness. Ivanov et al. (2009) incorporated a failure criterion within an FEA model to account for stiffness degradation and crack location. Li et al. (2009) developed a six subcell discretization approach of the RUC where each layer in the subcell was an integration point within a shell element layup. Goldberg et al. (2012) modified the through-thickness braiding approach by incorporating micromechanics and classical laminate theory to produce a homogenized shell element. Liu et al. (2011a; 2011b) developed a multiscale modeling approach using the GMC and a two-step homogenization process that introduced normal/shear coupling. Xiao et al. (2011) used a layered shell approach with a detailed subcell discretization method to account for different $V_f$ values for each subcell. Cater et al. (2013) created an absorbed matrix model, which was similar to the braiding through the thickness approach but accounted for intertow resin material, and was able to capture out-of-plane flexural properties. The absorbed matrix model also applied the different $V_f$ measurements to each subcell as well as the idealized tow shift rule.

### 1.5. Environmental Characterization

In the case of composite materials, the effect of environmental conditions is regarded as a limiting factor in mechanical performance (Adams & Singh, 1996; Bishop, 1985; Choi, Ahn, Nam, & Chun, 2001; Collings, Harvey, & Dalziel, 1993; Patel & Case, 2002). Therefore, an important and necessary step in the Federal Aviation Administration (FAA)
certification of aircraft designs is to determine the material integrity of engine components in relation to their mechanical performance under such extreme conditions. Woven and braided composites have been proven to have beneficial traits, such as delamination prevention, and are currently being used in aircraft structures. However, studies on braided composites are limited, when compared to the extensive durability studies currently available for unidirectional carbon/epoxy composites. For example, Bishop (1985) observed that elevated temperature conditions reduced the compressive failure strength of unidirectional carbon/epoxy composites. In addition to temperature, moisture studies using humidity-controlled chambers and circulating water baths have been conducted on unidirectional carbon/epoxy composites to determine their absorption behavior of (Choi et al., 2001; Suh, Ku, Nam, Kim, & Yoon, 2001). Joshi (1983) compared water bath and humidity-controlled experiments and concluded that water baths accelerated the moisture absorption in unidirectional composites. This study further illustrated how moisture absorption and elevated temperatures reduce the interlaminar shear strength by as much as 25% and the tensile strength by as much as 36%. The effect of moisture absorption on unidirectional carbon/epoxy composites has also been studied for tension and compression responses (Collings et al., 1993) and for the shear response (Adams & Singh, 1996). Patel and Case (2002) presented tension results for woven composites that were conditioned using hygrothermal cycling and moisture absorption, while Zhang et al. (2013) analyzed the reduction in tensile and compressive properties of triaxial braided composites due to microcracking induced by thermal cycling. Schambron et al. (2008) conditioned braided composite specimens in saline, moisture, and elevated temperature environments for bone plate structures and assessed the impact the conditioning had on the flexural properties.
Kohlman et al. (2011) performed hygrothermal cycling on triaxial braided composites to gauge the effect of environmental conditioning on tensile, compressive, and impact resistive properties. However, hygrothermal cycling cannot determine which specific stage (i.e., storage, ascent, cruise, or descent) is the most detrimental to the integrity of the composite material. Additional investigations, thus, are necessary to determine the effects of each individual environmental condition on the triaxial braid material, which is important for physics-based models and failure prediction.

1.5.1. Measurement Techniques for Triaxial Braided Composites

A variety of characterization techniques have been used to study the mechanical properties and damage in triaxial braided composites (Masters, Foye, Pastore, & Gowayed, 1993; Masters & Ifju, 1996; Portanova, 1995; Potluri, Manan, Francke, & Day, 2006; Roberts et al., 2009). Strain measurement systems, such as Moiré interferometry and digital image correlation (DIC), have been used extensively to characterize the full field strain of composite materials (Littell, Binienda, Roberts, & Goldberg, 2009; Masters & Ifju, 1996; Naik et al., 1994; Yekani Fard, Liu, & Chattopadhyay, 2011). Rao et al. (2002) used fiber Bragg grating (FBG) sensors on braided carbon/epoxy composites to measure the strain and temperature on the material. Quek et al. (2004) and Smith and Swanson (1994) tested triaxial braided composites using digital speckle photography to understand the failure modes of the material under biaxial loading. Correlations have been made between the strain field and damage assessment of composites using a combination of DIC and nondestructive scanning methods (Ivanov et al., 2009; Littell et al., 2009; Lomov et al., 2008). Flash thermography has been routinely used in recent studies to measure
specimen thickness, defects, and thermal diffusivity in large panels with no edge or boundary condition effects (Maldague, 2002; Shepard, Hou, Ahmed, & Lhota, 2006; J. G. Sun et al., 1997; Yekani Fard, Sadat, Raji, & Chattopadhyay, 2014). The main focus of these studies was to characterize mechanical properties and damage in complex composites.

1.6. Objectives of the Research

The overall purpose of the research presented in this dissertation is to experimentally characterize composite behavior and failure, and to develop a multiscale modeling framework in order to understand the effect of material variability and environmental conditions on the simulated response. The following are the main objectives of this work:

1. Characterize the local and spatial variability in unidirectional PMCs using statistical techniques to quantify microstructural parameters.

2. Develop stochastic micromechanics techniques capable of incorporating material variability, progressive damage, and failure theories at multiple length scales to improve the accuracy of material property and failure predictions.

3. Integrate progressive damage and multiscale failure theories within high fidelity micromechanics techniques to account for complex coupling between the composite constituents, including the fiber/polymer matrix interphase.

4. Perform experiments on triaxial braided PMCs to characterize the effect of various environmental conditions on the mechanical properties, damage, and failure of the material.
5. Develop a multiscale modeling framework capable of accounting for environmental conditions, 3D material architectures, and the scaling of the response to the structural level.

1.7. Outline of the Dissertation

The dissertation is structured as follows:

Chapter 2 presents the extension of a micromechanics theory, through the integration of stochastic methodologies, to create a modeling framework that is used to study the effect of material variability on the composite’s behavior and failure. Material variability is applied through the stochastic methodologies in the modeling framework by quantifying the local and spatial variability through a statistical, microstructural characterization of unidirectional composites. The model incorporates several theories, including viscoplastic, progressive damage, and multiscale failure laws. Additionally, a parametric study is performed using ballistic impact simulations of a PMC laminate to study the effect of material variability at the structural scale.

Chapter 3 integrates the progressive damage and multiscale failure theories from Chapter 2 with a high fidelity micromechanics technique that is capable of capturing complex coupling between the composite constituents. The high fidelity micromechanics also includes the fiber/polymer interphase, to observe the impact that the interphase has on the behavior and failure of the composite. Various interphase types and properties are applied to make a comparison of the simulated composite responses.

Chapter 4 characterizes the effect of environmental conditions on triaxial braided PMCs by conducting various tension, compression, and shear experiments. A major focus
of this study is determining the differences in local strain features caused by environmental conditions. The results from analyses of the tested specimens are provided to determine the influence of mechanical and environmental loading on the damage and failure modes.

Chapter 5 details the development of a multiscale modeling framework capable of simulating complex composite architectures and accounting for environmental conditions. Effective material properties, generated by high fidelity micromechanics with thermal and moisture expansion terms, are introduced into a mesoscale model which represents an RUC of triaxial braided composite material. The mesoscale is repeated to create a macroscale model where the material properties are defined with 3D material vectors to include out-of-plane components present in the physical material.

Chapter 6 summarizes the research reported in this dissertation and emphasizes its important contributions and findings. Potential areas and recommendations for future research work are also discussed at the end of the chapter.
2. MULTISCALE MODELING AND STOCHASTIC MICROMECHANICS FOR RATE-DEPENDENT COMPOSITE MATERIALS

2.1. Introduction

Damage initiation, damage evolution, and failure mechanisms in composites are complex and still an ongoing area of research. Multiphysics models with constitutive laws, progressive damage mechanics, and failure theories are required to capture the behavior and failure of composite structures subjected to complex loadings. The rate dependency and nonlinearity of PMCs further increase the complexity of the models required to simulate material behavior. Furthermore, certain material properties and geometric variabilities are inherent in composite materials due to the manufacturing and curing processes. It is necessary to quantify the effects of variability at every length scale in order to fully understand the impact on the structural response. Material variability may include variation in $V_f$, fiber dimensions, fiber waviness, and void distributions. Stochastic techniques are necessary to account for the aforementioned variability within a multiscale modeling framework. In this chapter, multiscale failure criteria, work potential damage mechanics, and material variability are incorporated within a stochastic sectional micromechanical model. The sectional micromechanics theory (Zhu, 2006; Zhu et al., 2006a, 2008) is utilized as it includes the rate dependency of the material and is computationally efficient due to the decoupling of the system of equations. The micromechanics model is capable of simulating 3D responses of the material including the through-thickness transverse shear and normal deformations. A modified Bodner-Partom viscoplastic theory (Goldberg et al., 2005) is used for the polymer constituents, and a 3D
progressive damage theory is derived to update the elastic material properties of the polymer constituent. Microstructural characterization is performed to understand the spatial variability in the composite material and develop statistical distributions for stochastic integration. The variabilities are integrated within the sectional micromechanics model using stochastic methodologies. Additionally, a multiple random variable analysis is performed using this stochastic micromechanics framework by using the $V_f$ characterization statistics and assuming small perturbations for the other random variable statistics.

2.1.1. **Sectional Micromechanics Theory**

The stochastic micromechanical model in this chapter is based on a 3D sectional micromechanical theory, which is a subcell based approach and accounts for 3D behavior of the material including in-plane deformation, transverse shear deformation, and through-thickness normal deformation. The sectional micromechanics is computationally efficient and preserves the transversely isotropic behavior of the composite unit cell. The theory and fundamental equations developed by Zhu et al. (2006; 2006a, 2008) are presented in this chapter for better understanding of the sectional micromechanics.

2.1.1.1. **Architecture and Discretization of the Unit Cell**

The discretization process in the sectional micromechanics, illustrated in Figure 2.1, defines the RUC of the composite as a single carbon fiber in a polymer matrix. The model assumes the composite material has square fiber packing and a perfect interfacial bond between the fiber and matrix. Due to the symmetry, a quarter of the unit cell is analyzed.
and, through the sectioning process, the large system of equations of the unit cell is decoupled into three smaller systems of equations. A system of equations is defined for each group of subcells (Groups A and B) and for the unit cell. A general solution methodology would require a system of equations comprising the constitutive equations and conditions for all eight subcells. However, the sectioning solution methodology allows each smaller system of equations to be solved independently to obtain the unit cell response, resulting in a significant reduction in computational cost.

The dimensions of each subcell are depicted in Figure 2.1 and are used to calculate the $V_f$ values for the subcell groups and the unit cell. The four lengths ($d_1$, $d_2$, $d_3$, and $d_4$) are specifically defined to preserve the transversely isotropic, material symmetry of the composite with the through-thickness length defined by a value of one. The lengths are determined using the following geometric assumptions:

$$d_1 + d_2 = \frac{\sqrt{2}}{2} R_f$$  \hspace{1cm} (2.1)
\[ d_1 + d_2 + d_3 = R_f \]  
\[ d_4 = 0.5 - R_f \]  
\[ 4(d_1 + d_2)^2 + 8(d_1)(d_3) = V_f \]

where \( V_f \) is the fiber volume fraction of the unit cell and \( R_f \) is the dimensionless radius of the carbon fiber calculated using Equation (2.5), which normalizes the lengths of the unit cell. Equation (2.4) represents the fiber volume fraction of the unit cell in terms of the dimensions of the rectangular subcells.

\[ R_f = \sqrt{\frac{V_f}{\pi}} \]  

The calculated rectangular subcell lengths are used to formulate Equation (2.6), which describe the variables applied to simplify the boundary and continuity conditions.

\[ hs_1 = 2d_1 \]
\[ hs_2 = 2d_2 \]
\[ hs_3 = 2d_3 \]
\[ hs_4 = 2d_4 \]
\[ hs_5 = \frac{d_1}{d_1 + d_2} \]
\[ hs_6 = \frac{d_2}{d_1 + d_2} \]
\[ hs_7 = \frac{d_3}{d_3 + d_4} \]
\[ hs_8 = \frac{d_4}{d_3 + d_4} \]
\[ hs_9 = 2(d_1 + d_2) \]
\[ hs_{10} = 2(d_3 + d_4) \]
The boundary and continuity conditions imposed by the micromechanics theory to solve the systems of equations for the unit cell and groups of subcells are described in the following subsections.

2.1.1.2. Stress and Strain Conditions for Group A

The continuity conditions are necessary to determine the effective stress and strain increments for Group A, and are expressed in Equations (2.7)-(2.12). The subscripts of the stress and strain increments in these expressions range from 1 to 6 and represent the Voigt notation of the parameters, and the superscripts in the parentheses (2, 3, 4, or A) represent either the subcell number or the group of subcells.

\[
\begin{align*}
  d\varepsilon_1^{(2)} &= d\varepsilon_1^{(3)} = d\varepsilon_1^{(4)} = d\varepsilon_1^{(A)} \\
  (h_s^1 h_s^7) d\sigma_1^{(2)} + (h_s^1 h_s^8) d\sigma_1^{(3)} + (h_s^1 h_s^7 + h_s^1 h_s^8) d\sigma_1^{(4)} &= d\sigma_1^{(A)} \\
  (h_s^3) d\sigma_2^{(2)} + (h_s^3) d\sigma_2^{(3)} &= d\sigma_2^{(A)} \\
  d\sigma_2^{(2)} &= d\sigma_2^{(3)} \\
  d\sigma_2^{(4)} &= d\sigma_2^{(A)} \\
  (h_s^3) d\varepsilon_2^{(2)} + (h_s^3) d\varepsilon_2^{(3)} &= d\varepsilon_2^{(A)} \\
  (h_s^6) d\sigma_3^{(2)} + (h_s^6) d\sigma_3^{(3)} &= d\sigma_3^{(A)} \\
  d\sigma_3^{(4)} &= d\sigma_3^{(A)} \\
  d\sigma_3^{(4)} &= d\sigma_3^{(3)} \\
  (h_s^5) d\varepsilon_3^{(2)} + (h_s^5) d\varepsilon_3^{(3)} &= d\varepsilon_3^{(A)} \\
  (h_s^5 h_s^7) d\gamma_4^{(2)} + (h_s^5 h_s^8) d\gamma_4^{(3)} + (h_s^5 h_s^7 + h_s^5 h_s^8) d\gamma_4^{(4)} &= d\gamma_4^{(A)} \\
\end{align*}
\]
\[ d\sigma_5^{(2)} = d\sigma_5^{(3)} = d\sigma_5^{(4)} = d\sigma_5^{(A)} \]
\[ (hs_5hs_7)d\gamma_5^{(2)} + (hs_5hs_8)d\gamma_5^{(3)} + (hs_6hs_7 + hs_6hs_8)d\gamma_5^{(4)} = d\gamma_5^{(A)} \]  
(2.11)

\[ (hs_6)d\sigma_6^{(4)} + (hs_5)d\sigma_6^{(3)} = d\sigma_6^{(A)} \]
\[ d\sigma_6^{(2)} = d\sigma_6^{(3)} \]
\[ d\gamma_6^{(A)} = d\gamma_6^{(A)} \]
\[ (hs_7)d\gamma_6^{(2)} + (hs_8)d\gamma_6^{(3)} = d\gamma_6^{(A)} \]  
(2.12)

2.1.1.3. Stress and Strain Conditions for Group B

Similar conditions are used to determine the effective stress and strain increments for Group B, and are expressed in Equations (2.13)-(2.18). In these expressions, the superscripts in the parentheses (5, 6, 7, or B) indicate either the subcell number or the group of subcells.

\[ d\varepsilon_1^{(5)} = d\varepsilon_1^{(6)} = d\varepsilon_1^{(7)} = d\varepsilon_1^{(B)} \]
\[ (hs_5hs_7)d\sigma_1^{(5)} + (hs_5hs_8)d\sigma_1^{(6)} + (hs_6hs_7 + hs_6hs_8)d\sigma_1^{(7)} = d\sigma_1^{(B)} \]  
(2.13)

\[ (hs_7)d\sigma_2^{(5)} + (hs_8)d\sigma_2^{(6)} = d\sigma_2^{(B)} \]
\[ d\sigma_2^{(2)} = d\sigma_2^{(3)} \]
\[ d\varepsilon_2^{(5)} = d\varepsilon_2^{(6)} \]
\[ (hs_6)d\varepsilon_2^{(7)} + (hs_8)d\varepsilon_2^{(6)} = d\varepsilon_2^{(B)} \]  
(2.14)

\[ (hs_6)d\sigma_3^{(7)} + (hs_8)d\sigma_3^{(6)} = d\sigma_3^{(B)} \]
\[ d\sigma_3^{(5)} = d\sigma_3^{(6)} \]
\[ d\varepsilon_3^{(5)} = d\varepsilon_3^{(6)} \]
\[ (hs_7)d\varepsilon_3^{(5)} + (hs_8)d\varepsilon_3^{(6)} = d\varepsilon_3^{(B)} \]  
(2.15)
\[ d\sigma_4^{(s)} = d\sigma_4^{(6)} = d\sigma_4^{(7)} = d\sigma_4^{(8)} \]
\[ (hs_s hs_s) d\gamma_4^{(s)} + (hs_s hs_s) d\gamma_4^{(6)} + (hs_s hs_s + hs_s hs_s) d\gamma_4^{(7)} = d\gamma_4^{(8)} \quad (2.16) \]

\[ (hs_s) d\sigma_5^{(7)} + (hs_s) d\sigma_5^{(6)} = d\sigma_5^{(8)} \]
\[ d\sigma_5^{(5)} = d\sigma_5^{(6)} \]
\[ d\gamma_5^{(7)} = d\gamma_5^{(8)} \]
\[ (hs_s) d\gamma_5^{(6)} + (hs_s) d\gamma_5^{(6)} = d\gamma_5^{(8)} \quad (2.17) \]

\[ d\sigma_6^{(5)} = d\sigma_6^{(6)} = d\sigma_6^{(7)} = d\sigma_6^{(8)} \]
\[ (hs_s hs_s) d\gamma_6^{(5)} + (hs_s hs_s) d\gamma_6^{(6)} + (hs_s hs_s + hs_s hs_s) d\gamma_6^{(7)} = d\gamma_6^{(8)} \quad (2.18) \]

### 2.1.1.4. Conditions and Equations for the Unit Cell

The incremental forms of stress and strain continuity conditions between the groups of subcells, described in Equations (2.19)-(2.24), are used to compute the unit cell response where the superscript \( u \) in parentheses denotes the strain or stress increment components of the unit cell.

\[ d\varepsilon_1^{(1)} = d\varepsilon_1^{(4)} = d\varepsilon_1^{(8)} = d\varepsilon_1^{(6)} = d\varepsilon_1^{(a)} \]
\[ (hs_s hs_s) d\sigma_1^{(1)} + (hs_s hs_s) d\sigma_1^{(4)} + (hs_s hs_s) d\sigma_1^{(8)} + (hs_s hs_s) d\sigma_1^{(8)} = d\sigma_1^{(a)} \quad (2.19) \]

\[ (hs_s) d\sigma_2^{(4)} + (hs_s) d\sigma_2^{(8)} = d\sigma_2^{(a)} \]
\[ d\sigma_2^{(8)} = d\sigma_2^{(8)} \]
\[ d\sigma_2^{(4)} = d\sigma_2^{(4)} \]
\[ (hs_s) d\varepsilon_2^{(8)} + (hs_s) d\varepsilon_2^{(8)} = d\varepsilon_2^{(a)} \]
\[ (hs_s) d\varepsilon_2^{(1)} + (hs_s) d\varepsilon_2^{(4)} = d\varepsilon_2^{(a)} \]

24
\[(h_s) d\sigma_3^{(b)} + (h_{s10}) d\sigma_3^{(u)} = d\sigma_3^{(u)}\]
\[d\sigma_3^{(A)} = d\sigma_3^{(b)}\]
\[d\sigma_3^{(I)} = d\sigma_3^{(u)}\]  
(2.21)

\[(h_s) d\varepsilon_3^{(A)} + (h_{s10}) d\varepsilon_3^{(b)} = d\varepsilon_3^{(u)}\]
\[(h_s) d\varepsilon_3^{(I)} + (h_{s10}) d\varepsilon_3^{(b)} = d\varepsilon_3^{(u)}\]

\[d\sigma_4^{(I)} = d\sigma_4^{(A)} = d\sigma_4^{(b)} = d\sigma_4^{(u)}\]
\[(h_s,h_{s10})d\gamma_4^{(I)} + (h_s,h_{s10})d\gamma_4^{(A)} + (h_{s10}h_{s10})d\gamma_4^{(b)} = d\gamma_4^{(u)}\]  
(2.22)

\[(h_s) d\sigma_5^{(b)} + (h_{s10}) d\sigma_5^{(u)} = d\sigma_5^{(u)}\]
\[d\sigma_5^{(A)} = d\sigma_5^{(b)}\]
\[d\sigma_5^{(I)} = d\sigma_5^{(u)}\]  
(2.23)

\[(h_s) d\gamma_5^{(A)} + (h_{s10}) d\gamma_5^{(b)} = d\gamma_5^{(u)}\]
\[(h_s) d\gamma_5^{(I)} + (h_{s10}) d\gamma_5^{(b)} = d\gamma_5^{(u)}\]

\[(h_s) d\sigma_6^{(A)} + (h_{s10}) d\sigma_6^{(u)} = d\sigma_6^{(u)}\]
\[d\sigma_6^{(b)} = d\sigma_6^{(u)}\]
\[d\sigma_6^{(I)} = d\sigma_6^{(u)}\]  
(2.24)

\[(h_s) d\gamma_6^{(b)} + (h_{s10}) d\gamma_6^{(u)} = d\gamma_6^{(u)}\]
\[(h_s) d\gamma_6^{(I)} + (h_{s10}) d\gamma_6^{(A)} = d\gamma_6^{(u)}\]

2.1.2. Work Potential Damage Law Overview

The progressive damage theory is based on a work potential model (Schapery, 1989, 1990; Schapery & Sicking, 1995), which is a thermodynamically consistent law that accounts for microscale damage by discretizing the total strain energy density, \(U\), into
components correlating to elastic strain energy density, $W_e$, and dissipated strain energy density, $W_d$, as shown in Equation (2.25).

$$ U = W_e + W_d $$

During loading, the structural changes and damage occurring within the material affect the elastic properties. The $W_e$ and $W_d$ variables are functions of internal state variables, $S_i$, where the subscript $i$ indicates that multiple internal state variables can be accounted for within the progressive damage law. These internal state variables represent separate types of structural changes and damage in the material. Equation (2.26) demonstrates that the differentiation of $W_d$ with respect to the general internal state variable, $S_i$, yields the thermodynamic force, $f_i$, required to produce the structural changes or damage associated with that internal state variable.

$$ f_i = \frac{\partial W_d}{\partial S_i} $$

Schapery (1989, 1990) showed that, through the definition and balance of thermodynamic forces, the total strain energy density is stationary with respect to the changes in the internal state variables that are associated with damage and structural changes as expressed in Equation (2.27). Rice (1971) showed that, according to the second law of thermodynamics, the energy expended for structural change or damage is irreversible with respect to time as depicted by Equation (2.28).

$$ \frac{\partial U}{\partial S_i} = 0 $$

$$ f_i \dot{S}_i \geq 0 $$

The work potential theory was further extended in a progressive damage theory developed by Pineda et al. (2009; 2012), where it was integrated with a GMC approach.
Considering only matrix microdamage, the strain energy density associated with damage can be represented using a single internal state variable, $S$. Therefore, following the differentiation scheme demonstrated in Equation (2.27) and differentiating Equation (2.25) with respect to $S$ yields

$$\frac{\partial W_e}{\partial S} = -1$$  \hspace{1cm} (2.29)$$

The elastic strain energy density for a composite plate, using plane stress conditions, is expressed as

$$W_e = \frac{1}{2}(E_{11}\varepsilon_{11}^2 + E_{22}\varepsilon_{22}^2 + G_{12}\gamma_{12}^2) + Q_{12}\varepsilon_{11}\varepsilon_{22}$$  \hspace{1cm} (2.30)$$

where the $Q_{12}$ variable is a component from a reduced stiffness matrix and is not dependent on structural changes. By substituting Equation (2.30) into Equation (2.29) and assuming that $E_{22}$ and $G_{12}$ are the only properties dependent on $S$, a differential equation is formulated (Equation (2.31)) for the evolution of damage.

$$\frac{\varepsilon_{22}^2}{2} \frac{\partial E_{22}}{\partial S} + \frac{\gamma_{12}^2}{2} \frac{\partial G_{12}}{\partial S} = -1$$  \hspace{1cm} (2.31)$$

The solution of Equation (2.31) is used to calculate the value of $S$, which is applied to the damage expression in Equation (2.32) to determine the degraded material property value.

$$P = P_0 p_d(S)$$  \hspace{1cm} (2.32)$$

The variable, $P$, can represent any material property, including transverse or in-plane shear moduli, and $P_0$ indicates the initial, undamaged value for the material property; and $p_d$ is an experimentally derived damage expression describing the degradation behavior as a function of $S$ for the specific material property. Sicking (1992) provided an experimental procedure for determining the damage expressions of the material properties, and
introduced a reduced damage parameter, $S_r$, (Equation (2.33)) to replace the original
damage variable, $S$, since the work showed that this substitution simplified the damage
expressions.

$$S_r = S^{1/3}$$

(2.33)

The substitution of the reduced damage parameter (Equation (2.33)) into Equation (2.31)
yields the following expanded form

$$\frac{\varepsilon_{22}^2}{2} \frac{\partial E_{22}}{\partial S_r} + \frac{\nu_{12}^2}{2} \frac{\partial G_{12}}{\partial S_r} = -3S_r^2$$

(2.34)

2.2. Variability Analysis

2.2.1. Local Microstructural Characterization

Characterization studies were conducted to understand the material microstructure and
to obtain the statistical distributions for the stochastic methodologies. Image quantification
was performed on unidirectional, carbon fiber reinforced PMC material using optical
microscopy (Zeiss LSM 700) to obtain the variability in the fiber volume fraction. Figure
2.2(a) shows a high magnification micrograph illustrating the microstructure for a PMC
laminate as well as the random location of the fibers within the polymer matrix. Multiple
micrographs were extracted from a local area of the composite to obtain a sufficient dataset.
A binary filter was applied to the micrographs in order to numerically distinguish the fiber
and the polymer matrix phases and accurately compute the $V_f$ statistics. The Bayesian
information criterion (BIC), presented in Equation (2.35), was used to determine the
optimal distribution type for each dataset (Schwarz, 1978). The BIC performs model
selection by implementing the likelihood function but also contains a penalty term to avoid over-fitting.

\[ BIC = -2 \ln L(\hat{\theta}_k | y) + k \ln c \]  

(2.35)

In Equation (2.35), \( L \) is the likelihood function, where \( \hat{\theta}_k \) represents the parameter values that maximize the likelihood function and \( y \) represents the observed data points. The variables \( k \) and \( c \) denote the number of free parameters and the number of data points contained in \( y \), respectively. Continuous distributions, such as the normal, extreme value, \( t \) location-scale, Weibull, and logistic distributions, were fitted to the data and the BIC was applied to determine the best fit distribution. For the local area \( V_f \) analysis, a normal distribution was found to be the best fit, and the probability density function is shown in Figure 2.2(b). The average and standard deviation parameters for the normal distribution are 63.9% and 2.21%, respectively. It must be noted that deterministic composite models use the average \( V_f \) to determine a periodic structure of the composite using a unit cell of a single fiber in a polymer matrix.

![Figure 2.2. PMC (a) Micrograph and (b) Probability Density Function for Fiber Volume Fraction](image)
2.2.2. Spatial Variability in Composite Microstructure

The distribution function plot in Figure 2.2(b) is a representation of the $V_f$ statistics obtained using high magnification micrographs randomly extracted from a local area, and an analysis of a larger area is needed in order to characterize the $V_f$ statistics and spatial variability for the entire composite laminate. Figure 2.3 shows a mosaic of the microstructure through-thickness for an eight layer unidirectional PMC. The mosaic is produced using the Zeiss image analysis software, which stitches several micrographs together creating a single, seamless image. The figure illustrates the spatial variability that occurs in the material where a region of the microstructure, for this particular specimen, contains areas of pure polymer matrix pockets and the rest of the microstructure contains tightly packed carbon fibers. Fiber volume fraction distributions were calculated from the microstructure for different sizes of boxed areas extracted from the mosaic. Different sized areas were used and randomly placed, and 50,000 measurements were made for each boxed area size. Figure 2.4 shows a series of distribution curves extracted using different sizes of boxed areas. Several distribution types were plotted for each boxed area size. For each legend in Figure 2.4, “empirical” represents the data calculated from the boxed areas, and the first distribution listed in the legend corresponds to the best fit distribution for that dataset. Similar to the local area analysis, continuous distributions were fitted, and the BIC was used to determine the best fit distribution and to rank the remaining distributions. The series of distribution plots shows that the $V_f$ distributions are unimodal in smaller boxed areas, and the distribution becomes bimodal as the size of the boxed areas increases. This trend in the distribution plots demonstrates the effect of the polymer matrix pockets, shown in the micrograph in Figure 2.3, and also the importance of using appropriate metrics for
microstructural characterization. For the region of polymer matrix pockets, when the boxed area size is small, the probability of the polymer matrix pockets being within the boxed areas is low. However, when the boxed area size increases, there is a higher probability that the polymer matrix pockets will be included in the boxed areas. The inclusion of the polymer matrix pockets causes the formation of a bimodal distribution. The distribution at the lower $V_f$ value represents the region containing the polymer matrix pockets.

Figure 2.3. Microstructure of an 8 Ply Unidirectional Composite Laminate
In order to account for the entire statistical distribution of the microstructural characterization data within the computational analysis, the polymer matrix pocket region in the large micrograph (Figure 2.3) was separated, and distribution plots were fitted for each separated region. Additionally, convergence studies were conducted to determine the appropriate number of boxed areas and boxed area sizes to accurately characterize the separated regions of the microstructure. The number of boxed areas was varied from 25 to
50,000, and $V_i$ values were calculated from a region away from the polymer matrix pocket region. The generalized extreme value distribution was determined to be the best fit for the collected data, and Figure 2.5(a) shows that the shape parameter of this statistical function converged at 20,000 boxed areas. This converged boxed area number was used in further analyses to define the converged dimensions for the boxed areas. Figure 2.5(b) shows that the best fit distribution function changes as the size of the boxed area changes and converges at an area of 300 µm by 300 µm. Using the parameters determined from the convergent studies, accurate distributions can be compiled for both the polymer matrix pocket region and the region away from the polymer matrix pockets (general composite region). Figure 2.6 displays the fitted distributions plots for these separated regions and the statistical parameter values for the best fit distributions are given in Table 2.1. The coefficient of variation (COV) is a normalized measure used to calculate the dispersion of a probability distribution. The distribution for the polymer matrix pocket region (Figure 2.6a) is shown to have a larger COV than the distribution for the general composite region (Figure 2.6b) due to the large uncertainty present in this region.
Figure 2.5. Convergence Study for a) Number of Boxed Areas and b) Size of the Boxed Areas

Table 2.1. Statistical Parameters for Microstructural Spatial Variability

<table>
<thead>
<tr>
<th></th>
<th>Shape</th>
<th>Scale</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polymer Matrix Pocket Region</td>
<td>0.0029</td>
<td>0.0156</td>
<td>0.6453</td>
</tr>
<tr>
<td>General Composite Region</td>
<td>-0.3640</td>
<td>0.0063</td>
<td>0.7022</td>
</tr>
</tbody>
</table>

Figure 2.6. Microstructural Characterization for a) Polymer Matrix Pocket Region and b) Region Away from the Polymer Matrix Pockets (General Composite Region)
2.3. Stochastic Micromechanical Model

2.3.1. Stochastic Techniques and Implementation

Stochastic methodologies are powerful techniques that can be integrated within modeling frameworks to incorporate material property scatter and microstructural variability. The following two stochastic methodologies have been investigated and compared in this work: the general Monte Carlo simulation (MCS) and the Latin hypercube sampling (LHS) based Monte Carlo technique. The LHS technique in this work discretizes the cumulative distribution function given for a random variable, and it randomly assigns a point within each discretized interval. By performing LHS, the distribution function can be defined with fewer samples compared to the MCS approach, which uses completely random sampling. The number of samples required for a stochastic methodology significantly affects the computational efficiency of the framework, as it is equivalent to the number of simulations performed using the sectional micromechanics model.

Using the local \( V_f \) analysis and statistics as an example, the stochastic methodology assigns the \( V_f \) as a random variable and uses it as an input into the sectional micromechanics. The best fit distribution for this particular \( V_f \) analysis correlated to a normal probability density function, \( f(x) \), described by Equation (2.36), and the cumulative distribution function, \( F(x) \), was calculated using the function in Equation (2.37).

\[
f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (2.36)
\]

\[
F(x) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{x-\mu}{\sqrt{2\sigma^2}} \right) \right] \quad (2.37)
\]
For Equations (2.36) and (2.37), $x$ is a manifested value of $V_f$, and the mean and standard deviation of the $V_f$ are shown as $\mu$ and $\sigma$, respectively. These cumulative distributions are continuous functions operating on a range of values from 0 to 1. This range is discretized using LHS through a set number of simulations, $N$. Examples of the general MCS and LHS methods (using $N = 20$ simulations) are shown in Figure 2.7, where one simulation represents a single value of $V_f$. For the MCS technique, the random sampling of the cumulative distribution function for the $V_f$ is sparse on the right portion of the plot, while the LHS represents the entire distribution well and randomness is still captured within the discretized intervals. The points computed within these intervals represent cumulative distribution function values, and Equation (2.37) can be inverted to calculate $V_f$ values.

For multiple random parameters in the LHS method, a single representation of the $V_f$ is randomly paired with the other parameter and arranged into parameter sets. This pairing of parameter sets is demonstrated in Figure 2.8, where the index column of the table signifies the data for the random variables, and “X” indicates the value used for each parameter for that particular set. Additionally, an advanced pairing rule is used in this work to force the pairing process to only allow one value from each row in the table for a single parameter set, which enables better representation of the entire distribution for each random parameter. The sampled set of material parameters is used as inputs for the sectional micromechanics model. A different sampled set of material parameters is used for each simulation of the model until $N$-number of stress-strain curves are obtained (Figure 2.9).
Figure 2.7. Cumulative Distribution Functions of $V_f$ with (a) General MCS and (b) LHS Based Monte Carlo

<table>
<thead>
<tr>
<th>Index #</th>
<th>$V_f$</th>
<th>$Z$</th>
<th>...</th>
<th>$ith$ variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td>$X$</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>$X$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>$X$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Input Variables for First Run: $V_f(4)$, $Z(2)$, ...

Figure 2.8. Latin Hypercube Selection Process
2.3.2. 3D Progressive Damage Theory

The work potential damage theory, detailed at the beginning of this chapter (Chapter 2.1.2), is integrated within the stochastic sectional micromechanical theory. A 3D form of the progressive damage theory is applied to the polymer subcells. Microdamage of the polymer is assumed to affect only the elastic modulus of the polymer constituent, and the generalized damage equation is shown in Equation (2.38). A third order polynomial is used to describe the damage function in this work, and the coefficients in Table 2.2 are defined based on a similar function shown in Pineda et al. (2009).

\[ p_d(S_r) = p_0 + p_1 S_r + p_2 S_r^2 \cdots + p_n S_r^n \]  

(2.38)
Since the current progressive damage theory is a 3D derivation, the elastic strain energy density is defined by

\[
W_e = \frac{1}{2} \left( E_{11} \varepsilon_{11}^2 + E_{22} \varepsilon_{22}^2 + E_{33} \varepsilon_{33}^2 + G_{12} \gamma_{12}^2 + G_{13} \gamma_{13}^2 + G_{23} \gamma_{23}^2 \right)
\]  

(2.39)

Assuming isotropic behavior in the polymer, Equation (2.39) can be reduced to

\[
W_e = \frac{1}{2} E_m \left( \varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2 \right) + \frac{E_m}{4(1 + v_m)} \left( \gamma_{12}^2 + \gamma_{13}^2 + \gamma_{23}^2 \right)
\]  

(2.40)

By substituting Equation (2.40) into Equation (2.29), the differential equation describing the damage evolution is expressed as

\[
\frac{\partial W_e}{\partial \varepsilon} = \frac{1}{2} \frac{\partial E_m}{\partial \varepsilon} \left( \varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2 \right) + \frac{1}{4(1 + v_m)} \frac{\partial E_m}{\partial \gamma} \left( \gamma_{12}^2 + \gamma_{13}^2 + \gamma_{23}^2 \right) = -1
\]  

(2.41)

and the substitution of the reduced damage parameter (Equation (2.33)) into Equation (2.41) for yields

\[
\frac{1}{2} \frac{\partial E_m}{\partial \varepsilon} \left( \varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2 \right) + \frac{1}{4(1 + v_m)} \frac{\partial E_m}{\partial \gamma} \left( \gamma_{12}^2 + \gamma_{13}^2 + \gamma_{23}^2 \right) = -3S_r^2
\]  

(2.42)

<table>
<thead>
<tr>
<th>Table 2.2. Damage Function Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient</td>
</tr>
<tr>
<td>p0</td>
</tr>
<tr>
<td>p1</td>
</tr>
<tr>
<td>p2</td>
</tr>
<tr>
<td>p3</td>
</tr>
</tbody>
</table>

2.3.3. Constitutive Laws

The incremental constitutive equations for the fiber subcells are represented by a transversely isotropic, linear elastic model (Equation (2.43)) with the compliance tensor,
\( S' \), represented in Equation (2.44), where the variables \( d\varepsilon^f \) and \( d\sigma^f \) represent the strain and stress increments of the fiber subcells, respectively. The elastic material properties for the fiber constituent used in this model are presented in Table 2.3.

\[
d\varepsilon_i^f = S_{ij}^f d\sigma_j^f \quad i, j = 1 \cdots 6 \tag{2.43}
\]

\[
S^f = \begin{bmatrix}
\frac{1}{E_1^f} & -\nu_{21}^f & 0 & 0 & 0 \\
\frac{-\nu_{21}^f}{E_2^f} & \frac{1}{E_2^f} & 0 & 0 & 0 \\
\frac{-\nu_{12}^f}{E_1^f} & \frac{-\nu_{32}^f}{E_2^f} & \frac{1}{E_2^f} & 0 & 0 \\
0 & 0 & \frac{1}{G_{23}^f} & 0 & 0 \\
0 & 0 & 0 & \frac{1}{G_{12}^f} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_{12}^f}
\end{bmatrix}
\tag{2.44}
\]

Table 2.3. IM7 Carbon Fiber Material Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_{11} ) (GPa)</td>
<td>276</td>
</tr>
<tr>
<td>( E_{22} ) (GPa)</td>
<td>13.8</td>
</tr>
<tr>
<td>( G_{12} ) (GPa)</td>
<td>20</td>
</tr>
<tr>
<td>( G_{23} ) (GPa)</td>
<td>5.52</td>
</tr>
<tr>
<td>( \nu_{12} )</td>
<td>0.25</td>
</tr>
<tr>
<td>( \nu_{23} )</td>
<td>0.25</td>
</tr>
<tr>
<td>( \rho ) (kg/m(^3))</td>
<td>1800</td>
</tr>
</tbody>
</table>

The constitutive law for the polymer subcells incorporates a viscoplastic state variable model developed by Goldberg et al. (2005) and the theory is presented here. This
constitutive model is based on the Bodner-Partom viscoplastic state variable model, which was originally developed to analyze the viscoplastic deformation of metals above one-half of the melting temperature (Bodner, 2002). Previous studies have demonstrated that the hydrostatic stress of the polymer material is an important factor in describing the material behavior (Ward & Sweeney, 2012). Therefore, Goldberg et al. (2005) modified the viscoplastic constitutive model by integrating hydrostatic stress effects to capture the nonlinear behavior of PMC materials using a micromechanical model with a range of applied strain rates. This modified viscoplastic constitutive law is applied to the modeling framework in this chapter, and the viscoplastic derivation uses the inelastic potential function defined in Equation (2.45), which is based on the Drucker-Prager yield criterion (Khan & Huang, 1995).

\[ f = \sqrt{J_2} + \alpha \sigma_{kk} \]  
(2.45)

In Equation (2.45), \( J_2 \) is the second invariant of the deviatoric stress tensor, \( \alpha \) is an internal state variable that controls the level of hydrostatic stress effects, and \( \sigma_{kk} \) is the first invariant of the stress tensor. The components of the inelastic strain rate tensor, \( \dot{\varepsilon}_{ij}^l \), in Equation (2.46) are dependent on the scalar rate of the plastic multiplier, \( \dot{\lambda} \), and on the partial derivative of the inelastic potential function from Equation (2.45) with respect to the stress tensor components.

\[ \dot{\varepsilon}_{ij}^l = \dot{\lambda} \frac{\partial f}{\partial \sigma_{ij}} \]  
(2.46)

The solution for the partial derivative in Equation (2.46) yields

\[ \frac{\partial f}{\partial \sigma_{ij}} = \frac{\sigma_{ij}^{dev}}{2\sqrt{J_2}} + \alpha \delta_{ij} \]  
(2.47)
where $\sigma_{ij}^{\text{dev}}$ contains the deviatoric stress components and $\delta_{ij}$ is the Kronecker delta. Utilizing the principal of the equivalence for the inelastic work rate shows that $\lambda$ is defined by

$$\dot{\lambda} = \sqrt{3} \dot{\varepsilon}_e^I$$

(2.48)

Therefore, $\dot{\varepsilon}_e^I$ can be determined by following a similar derivation to the Bodner-Partom model (Bodner, 2002), and the final form can be expressed as

$$\dot{\varepsilon}_e^I = 2D_0 \exp \left[-\frac{1}{2} \left(\frac{Z}{\sigma_e}\right)^{2n}\right] \left[\frac{\sigma_{ij}^{\text{dev}}}{2\sqrt{J_2}} + \alpha \delta_{ij}\right]$$

(2.49)

where $n$ controls the rate dependence of the material, $Z$ is a variable related to the resistance of molecular flow, and $D_0$ is the maximum inelastic strain rate. Additionally, the effective stress, $\sigma_e$, is defined as

$$\sigma_e = \sqrt{3} f = \sqrt{3} J_2 + \sqrt{3} \alpha \sigma_{kk}$$

(2.50)

The evolution rate for the internal state variables, $Z$ and $\alpha$, are expressed in Equations (2.51) and (2.52), respectively, where the effective deviatoric inelastic strain rate, $\dot{\varepsilon}_e^I$, is defined using Equations (2.53) and (2.54). $Z_l$ and $\alpha_l$ represent the maximum values for their respective parameters, whereas $Z_0$ and $\alpha_0$ represent the initial values.

$$\dot{Z} = q(Z_l - Z) \dot{\varepsilon}_e^I$$

(2.51)

$$\dot{\alpha} = q(\alpha_l - \alpha) \dot{\varepsilon}_e^I$$

(2.52)

$$\dot{\varepsilon}_e^I = \sqrt{\frac{2}{3} \varepsilon_{ij}^I \varepsilon_{ij}^I}$$

(2.53)

$$\varepsilon_{ij}^I = \varepsilon_{ij}^I - \varepsilon_{im}^I \delta_{mj}$$

(2.54)
The effective inelastic strain rate, $\dot{\varepsilon}_e^I$, is equivalent to the effective deviatoric inelastic strain rate, $\dot{\varepsilon}_e^I$, due to the assumption of plastic incompressibility (Fleck & Hutchinson, 2001). This viscoplastic model was incorporated within the incremental constitutive equations for the polymer subcells (Equation (2.55)).

$$d\varepsilon_i^m = S_{ij}^m d\sigma_j^m + d\varepsilon_i^I, \quad i, j = 1\ldots6$$ (2.55)

In Equation (2.55), the variables $d\varepsilon_i^m$ and $d\sigma_j^m$ represent the strain and stress increments of the polymer matrix subcells, respectively, and $S_{ij}^m$ contains the components of the compliance tensor for the polymer matrix subcells. $d\varepsilon_i^I$ is the inelastic strain increment of the polymer matrix subcells obtained using Equation (2.49). The compliance tensor for the polymer subcells is updated using the calculated damage parameter, $p_d$, from the 3D progressive damage theory, and the Voigt notation of this tensor is described in Equation (2.56). The elastic and inelastic material properties for the polymer matrix constituent are presented in Table 2.4. It is important to note that previous studies have shown that the polymer’s elastic modulus is rate-dependent (Gilat, Goldberg, & Roberts, 2002; Zhu, 2006); therefore, three values are given for the modulus. The individual subcell strain rate is calculated, and interpolation is used to designate an appropriate modulus for each subcell.

$$S_{ij}^m = \frac{1}{p_d E_m}$$

\[
S_{ij}^m = \begin{bmatrix}
1 & -\nu^m & -\nu^m & 0 & 0 & 0 \\
-\nu^m & 1 & -\nu^m & 0 & 0 & 0 \\
-\nu^m & -\nu^m & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 2(1+\nu) & 0 & 0 \\
0 & 0 & 0 & 0 & 2(1+\nu) & 0 \\
0 & 0 & 0 & 0 & 0 & 2(1+\nu) \\
\end{bmatrix} \] (2.56)
### Table 2.4. Material Properties for 977-2 Epoxy

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>$3.52$ ($\dot{\varepsilon} = 9 \times 10^{-5}$ s$^{-1}$)</td>
</tr>
<tr>
<td></td>
<td>$3.52$ ($\dot{\varepsilon} = 1.90$ s$^{-1}$)</td>
</tr>
<tr>
<td></td>
<td>$6.33$ ($\dot{\varepsilon} = 500$ s$^{-1}$)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$0.4$</td>
</tr>
<tr>
<td>$D_0$</td>
<td>$1.00 \times 10^6$</td>
</tr>
<tr>
<td>$n$</td>
<td>$0.852$</td>
</tr>
<tr>
<td>$Z_0$ (MPa)</td>
<td>$259.496$</td>
</tr>
<tr>
<td>$Z_1$ (MPa)</td>
<td>$1131.371$</td>
</tr>
<tr>
<td>$q$</td>
<td>$150.498$</td>
</tr>
<tr>
<td>$\alpha_0$</td>
<td>$0.129$</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>$0.152$</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>$1310$</td>
</tr>
</tbody>
</table>

### 2.3.4. Multiscale Failure Criteria

The failure of individual polymer subcells was accounted for by incorporating a microscale maximum strain failure criterion. The maximum strain criterion is expressed in Equations (2.57)-(2.62), where the superscript $s$ indicates the subcell being analyzed for failure and the local subcell strain is determined within the sectional micromechanics. Additionally, the superscript $u$ indicates the ultimate strain parameter, and the subscripts $t$ and $c$ denote whether the loading is tension or compression, respectively.

\[
\varepsilon_1^{(s)} = \begin{cases} 
\varepsilon_{1t}^u & \text{when } \varepsilon_1^{(s)} > 0 \\
\varepsilon_{1c}^u & \text{when } \varepsilon_1^{(s)} < 0 
\end{cases} \quad (2.57)
\]

\[
\varepsilon_2^{(s)} = \begin{cases} 
\varepsilon_{2t}^u & \text{when } \varepsilon_2^{(s)} > 0 \\
\varepsilon_{2c}^u & \text{when } \varepsilon_2^{(s)} < 0 
\end{cases} \quad (2.58)
\]

\[
\varepsilon_3^{(s)} = \begin{cases} 
\varepsilon_{3t}^u & \text{when } \varepsilon_3^{(s)} > 0 \\
\varepsilon_{3c}^u & \text{when } \varepsilon_3^{(s)} < 0 
\end{cases} \quad (2.59)
\]
\[
\left| \psi_4^{(i)} \right| = \gamma_4^u \\
\left| \psi_5^{(i)} \right| = \gamma_5^u \\
\left| \psi_6^{(i)} \right| = \gamma_6^u
\] 

(2.60)  
(2.61)  
(2.62)

If the local strain in the subcell exceeds the ultimate strain, then failure is indicated and the stress component for that specific direction is set to zero. The failure properties for the polymer matrix used in this modeling framework are stated in Table 2.5. It is important to note that Gilat et al. (2002) has shown that the tensile failure properties for 977-2 epoxy are rate-dependent. Additionally, the compressive and shear failure properties applied to this criterion are assigned values based on similar experiments and polymer materials from Goldberg et al. (2003).

<table>
<thead>
<tr>
<th>( \varepsilon ) (s(^{-1}))</th>
<th>( \varepsilon_t^u )</th>
<th>( \varepsilon_c^u )</th>
<th>( \gamma_c^u )</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.5E-5</td>
<td>0.045</td>
<td>0.07</td>
<td>0.125</td>
</tr>
<tr>
<td>1.30</td>
<td>0.032</td>
<td>0.07</td>
<td>0.125</td>
</tr>
<tr>
<td>360</td>
<td>0.019</td>
<td>0.07</td>
<td>0.125</td>
</tr>
</tbody>
</table>

Table 2.5. Failure Strains for 977-2 Epoxy

The macroscale failure criteria are based on a modified Hashin failure theory (Zhu et al., 2008) that incorporates the shear stress effect in the compressive fiber failure mode, which was not considered in the original Hashin failure theory (Hashin, 1980). Equations (2.63) and (2.64) describe the failure criteria for the fiber mode in tension and compression,
respectively. Equations (2.65) and (2.66) describe the failure criteria for the polymer mode in tension and compression, respectively.

\[
\begin{aligned}
\left\lfloor \frac{\sigma_{11}}{\sigma_A^+} \right\rfloor^2 + \frac{1}{\tau_A^+} \left( \sigma_{12}^2 + \sigma_{13}^2 \right) &= 1 \\
\sigma_{11} &> 0
\end{aligned}
\]  

\[
\begin{aligned}
\left\lfloor \frac{\sigma_{11}}{\sigma_A^-} \right\rfloor^2 + \frac{1}{\tau_A^-} \left( \sigma_{12}^2 + \sigma_{13}^2 \right) &= 1 \\
\sigma_{11} &< 0
\end{aligned}
\]  

\[
\begin{aligned}
\frac{1}{\left(\sigma_T^+\right)^2} \left( \sigma_{22} + \sigma_{33} \right) &+ \frac{1}{\tau_T^+} \left( \sigma_{23}^2 - \sigma_{22} \sigma_{33} \right) \\
&\quad + \frac{1}{\tau_A^-} \left( \sigma_{12}^2 + \sigma_{13}^2 \right) = 1
\end{aligned}
\]  

\[
\begin{aligned}
\frac{1}{\sigma_T^+} \left[ \frac{\left(\sigma_T^+\right)^2}{2\tau_T^+} \right] - 1 \left( \sigma_{22} + \sigma_{33} \right) &+ \frac{1}{4\tau_T^+} \left( \sigma_{22} + \sigma_{33} \right)^2 \\
&\quad + \frac{1}{\tau_T^-} \left( \sigma_{23}^2 - \sigma_{22} \sigma_{33} \right) + \frac{1}{\tau_A^+} \left( \sigma_{12}^2 + \sigma_{13}^2 \right) = 1
\end{aligned}
\]  

The four failure modes are formulated as functions of the failure strengths of the composite material. The parameters \( \sigma_A^+ \) and \( \sigma_A^- \) represent the tensile and compressive failure strengths in the fiber direction, respectively. The parameters \( \sigma_T^+ \) and \( \sigma_T^- \) represent the tensile and compressive failure strengths perpendicular to the fiber direction, respectively.
The parameters $\tau_T$ and $\tau_A$ represent the transverse and axial shear strengths, respectively.

Similar to the subcell failure criterion, several failure parameters for the composite are strain rate-dependent. The failure strength values in Table 2.6 are obtained from the experimental data given by Goldberg et al. (2003).

<table>
<thead>
<tr>
<th>$\dot{\varepsilon}$ (s$^{-1}$)</th>
<th>$\sigma_A^+$ (MPa)</th>
<th>$\sigma_T^+$ (MPa)</th>
<th>$\sigma_A^-$ (MPa)</th>
<th>$\sigma_T^-$ (MPa)</th>
<th>$\tau_T$ (MPa)</th>
<th>$\tau_A$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.75E-5</td>
<td>2300</td>
<td>75</td>
<td>900</td>
<td>150</td>
<td>66.46</td>
<td>86</td>
</tr>
<tr>
<td>1.9</td>
<td>2300</td>
<td>85</td>
<td>900</td>
<td>170</td>
<td>66.46</td>
<td>112</td>
</tr>
<tr>
<td>500</td>
<td>2300</td>
<td>100</td>
<td>900</td>
<td>200</td>
<td>66.46</td>
<td>132</td>
</tr>
</tbody>
</table>

2.4. Impact Model Development

A multiscale model consisting of the sectional micromechanics and Hashin failure theory was integrated in a user defined material subroutine within the LS-DYNA nonlinear FEA software to simulate the impact behavior of a PMC laminate under various loading conditions. A parametric study was performed to determine the variability in laminate impact simulations. The $V_f$ and initial velocity were the designated parameters for the study. The laminated circular plate was 200 mm in diameter and comprised of four IM7/977-2 unidirectional laminae with a [0$_4$] stacking sequence and lamina thickness of 0.5 mm. A fixed boundary condition was applied to the nodes on the circumference of the composite laminate. The steel projectile measured 40 mm in diameter and 80 mm in length, and was modeled as an elastic material. The plate and projectile were meshed using brick elements with a single integration point per element for improved computational efficiency. Mesh refinement was implemented in the central region of the composite plate.
near the impact location due to the presence of large stress and strain gradients caused by the high strain rate impact event. The meshed composite plate and projectile geometries are presented in Figure 2.10. The number of elements used in the model was 6496 elements for the composite laminate and 320 elements for the steel projectile. The dynamic simulations were executed with explicit time integration using adaptive time steps. An eroding contact card was defined in LS-DYNA and coupled with the failure model to accurately account for the elements that were no longer able to carry load. The element erosion was determined by the previously described Hashin failure criteria. When an element failed it was deleted and the contact surfaces were automatically updated.

Figure 2.10. Meshed Geometries for Impact Simulation

2.5. Results and Discussion

2.5.1. Comparison of Stochastic Methodologies

A comparison of the general MCS and the LHS based Monte Carlo methodologies was conducted to investigate the accuracy and efficiency of each method. The statistical
distribution parameters for the $V_t$ were calculated using the normal distribution from the local area analysis, where the mean and standard deviation parameter values were 63.90% and 2.21%, respectively. Figure 2.11 shows the stochastic transverse tensile response for both the LHS and MCS techniques using a small number of simulations ($N = 20$). These results demonstrate that, even with a small number of simulations, the LHS methodology can capture a larger variation in response compared to the MCS results. However, an appropriate number of simulations is needed to accurately compare the stochastic methodologies. In order to achieve convergence, the transverse failure strength and failure strain were considered, and the resulting COV values are shown in Figure 2.12. Both general MCS and LHS based Monte Carlo are displayed in these plots. A key distinction in Figure 2.12 is that the converged value for the transverse strength COV is approximately 0.28%, while the COV for the transverse strain is 1.95%. Therefore, the transverse failure strain exhibits a larger dispersion of the variability compared to the transverse failure strength due to the assumed random variables. Analysis shows that while both methods converged at approximately the same COV value, the LHS converged in a fewer number of simulations. The COV value was assumed to have already converged by a simulation count of 1,000, with convergence being defined as the point in which the difference in COV values was consistently within 3%. Specifically, the LHS technique required 100 simulations for convergence. The calculated advantage of using the LHS method over the MCS is demonstrated by a comparison of the set of results which that LHS converges with 80% fewer simulations when analyzing the COV trend of the failure stress plot and 95% fewer simulations when using the COV trend of the failure strain plot.
Figure 2.11. In-Plane Transverse Response using (a) LHS and (b) General MCS

Figure 2.12. Comparison of COV with Varying Number of Simulations for MCS and LHS Showing (a) Transverse Failure Strain and (b) Transverse Failure Strength

2.5.2. Stochastic Results using Microstructure Variability

The effect of the microscale, macroscale, and work potential damage theories on the model were studied, and deterministic results are shown in Figure 2.13. The figure shows the deterministic, transverse tensile response loaded using a strain rate of 1.05 s\(^{-1}\). For the figure legends and tabulated results, “Macro” refers to the model with only the modified
Hashin criteria applied; “Damage/Macro” refers to the model with the microscale damage theory as well as the modified Hashin criteria; and “Damage/Micro/Macro” indicates the full combination of the microscale damage and multiscale failure criteria. The modeling curves were compared with the experimental data obtained by Gilat et al. (2002). The figure shows that, by introducing the microscale failure theory and damage theory, the current Damage/Micro/Macro model is able to capture the experimental transverse tensile behavior more accurately compared to the original model, which only considers the macroscale failure using the modified Hashin criteria.

Figure 2.13. Micromechanical Low Strain Rate (1.05 s⁻¹) Results for Multiple Deterministic Models Compared with Experimental Data (Gilat et al., 2002)

The stochastic response was investigated using the spatial $V_f$ variability by performing simulations using the distribution statistics from Table 2.1. The results were obtained by
discretizing the distribution functions using 100 simulations, since the convergence study in Chapter 4.3.1 showed that this number of simulations is sufficient when using the LHS methodology. Figure 2.14(a) shows the effect of the variability in the polymer matrix pocket region on the transverse stress-strain behavior. The general composite region of the laminate’s microstructure was also simulated, and the results are shown in Figure 2.14(b). A comparison between the stochastic, transverse tensile simulation results using the distribution functions for the local area analysis, polymer matrix pocket region, and general composite region is presented Table 2.7. The error analysis results in this table are obtained through comparison with the available experimental data referred to previously. The material parameters shown in the table are the simulated failure strain, failure strength, and modulus as these three parameters represent the behavior and failure of the material. Since the experimental data consists of a single curve, the minimum error value is the best error measure for stochastic results, as it represents the probability of one of the stochastic curves being the same as the experimental curve; whereas the average error value better represents the trend of the data. There is less variation in the general composite response because the COV of the characterized distributions for the general composite region is less than that of the polymer matrix pocket region. The percent differences also show that the stochastic simulation of the general composite region has a lower COV than the results from the polymer matrix pocket region. The minimum percentage differences in the table shows that failure strain of the general composite region correlates best with the experimental failure strain and the modulus of the polymer matrix pocket region has a better correlation with the experimental modulus. Additionally, as observed in Figure 2.14, the simulation
results from the general composite region yield higher transverse stiffness moduli due to the larger amount of polymer matrix in the polymer matrix pocket region.

Figure 2.14. Stochastic Transverse Tensile Responses using Statistical Data from (a) the Polymer Matrix Pocket Region and (b) the General Composite Region
Table 2.7. Transverse Tensile Experimental Comparison of Variability

<table>
<thead>
<tr>
<th></th>
<th>Local</th>
<th>Polymer Pocket Region</th>
<th>General Region</th>
<th>Deterministic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min. Difference - Failure Strain [%]</td>
<td>10.32</td>
<td>10.30</td>
<td>5.58</td>
<td>18.40</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strain [%]</td>
<td>21.55</td>
<td>21.43</td>
<td>9.64</td>
<td>18.40</td>
</tr>
<tr>
<td>COV - Failure Strain [%]</td>
<td>4.68</td>
<td>4.66</td>
<td>1.56</td>
<td>n/a</td>
</tr>
<tr>
<td>Min. Difference - Failure Strength [%]</td>
<td>15.44</td>
<td>15.39</td>
<td>15.46</td>
<td>15.63</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strength [%]</td>
<td>15.59</td>
<td>15.61</td>
<td>15.59</td>
<td>15.63</td>
</tr>
<tr>
<td>COV - Failure Strength [%]</td>
<td>0.09</td>
<td>0.08</td>
<td>0.08</td>
<td>n/a</td>
</tr>
<tr>
<td>Min. Difference - Modulus [%]</td>
<td>0.05</td>
<td>0.06</td>
<td>1.06</td>
<td>5.07</td>
</tr>
<tr>
<td>Avg. Difference - Modulus [%]</td>
<td>9.70</td>
<td>9.73</td>
<td>5.17</td>
<td>5.07</td>
</tr>
<tr>
<td>COV - Modulus [%]</td>
<td>4.71</td>
<td>4.74</td>
<td>1.55</td>
<td>n/a</td>
</tr>
</tbody>
</table>

Figure 2.15 and Figure 2.16 show the modeled response due to in-plane and out-of-plane shear loading, respectively, for a strain rate of 1.05 s⁻¹, and the results are compared to deterministic MAC/GMC simulations (Bednarcyk & Arnold, 2002b; Zhu, 2006). The spatial $V_f$ variability distributions are utilized in the simulations depicted in both figures and the MAC/GMC simulations use a unit cell discretization of 18 by 18 subcells. The polymer matrix pocket region is shown to have better correlation with the MAC/GMC results for both the in-plane shear and out-of-plane shear responses. Through the incorporation of stochastic methodologies, the figures show that the variability in $V_f$ has a larger effect on the in-plane shear response. It is also important to note that there is a larger variation in the response under shear loading compared to the transverse tensile loading.
Figure 2.15. Stochastic In-Plane Shear Responses using Statistical Data from (a) the Polymer Matrix Pocket Region and (b) the General Composite Region
Figure 2.16. Stochastic Out-of-Plane Shear Responses using Statistical Data from (a) the Polymer Matrix Pocket Region and (b) the General Composite Region.
2.5.3. Stochastic Results for Multiple Random Variables

The results from the previous section aptly demonstrate the effect of $V_f$ variability on the material response. Therefore, the investigation is extended to study the effects of variability on the composite response using combinations of other material properties. The statistical distribution for the local area characterization of the $V_f$ was used, and normal distributions were assigned for several polymer matrix material properties ($Z$, $n$, and $E_m$) as shown in Table 2.8. These assumed standard deviation values for the random polymer variables were used to determine the capability of the stochastic framework to properly incorporate multiple random variables, and additional experimentation is recommended to obtain these parameters. Figure 2.17 illustrates the stochastic in-plane shear response from applying the $V_f$ and $Z$ parameters as random variables, and these results show that the variation in response becomes larger as the number of random variables increases. Error analysis was performed for multiple random variable analyses, and the results are presented in Table 2.9 and Table 2.10 as average and minimum percent difference values using the experimental data as a reference. Table 2.9 presents a comparison of the stochastic sectional model using only the Hashin failure criteria from the original sectional micromechanics model (Zhu, 2006; Zhu, Chattopadhyay, & Goldberg, 2006a, 2008). There is a minimal decrease in the average error values of the statistical parameters as multiple random variables are introduced, but a large decrease in the minimum error is observed for failure strain and modulus as multiple random variables are added. The entries in Table 2.10 compare stochastic results from different combinations of the damage and failure theories using all four random parameters. A small increase in minimum error
is observed for failure strain and failure strength, but there is a significant decrease in the minimum error for the modulus.

Table 2.8. Multiple Random Variable Statistics

<table>
<thead>
<tr>
<th></th>
<th>$V_f$ (%)</th>
<th>$Z$ (Pa)</th>
<th>$n$</th>
<th>$E_m$ (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard Deviation</td>
<td>2.21</td>
<td>1.08E7</td>
<td>0.0325</td>
<td>0.99E8</td>
</tr>
<tr>
<td>Average</td>
<td>63.90</td>
<td>2.59E8</td>
<td>0.8515</td>
<td>3.52E9</td>
</tr>
</tbody>
</table>

Figure 2.17. Stochastic In-Plane Shear Response using LHS for (a) the $Z$ Variable Distribution and (b) the $V_f$ and $Z$ Distribution
Table 2.9. Experimental Comparison of Multiple Random Variables

<table>
<thead>
<tr>
<th></th>
<th>Random Variables:</th>
<th>Deterministic:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$V_f$</td>
<td>$V_f$ &amp; $Z$</td>
</tr>
<tr>
<td>Min. Difference - Failure Strain [%]</td>
<td>11.14</td>
<td>10.81</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strain [%]</td>
<td>17.30</td>
<td>17.31</td>
</tr>
<tr>
<td>COV - Failure Strain [%]</td>
<td>1.99</td>
<td>2.00</td>
</tr>
<tr>
<td>Min. Difference - Failure Strength [%]</td>
<td>12.36</td>
<td>12.27</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strength [%]</td>
<td>12.97</td>
<td>12.96</td>
</tr>
<tr>
<td>COV - Failure Strength [%]</td>
<td>0.26</td>
<td>0.28</td>
</tr>
<tr>
<td>Min. Difference - Modulus [%]</td>
<td>25.41</td>
<td>24.71</td>
</tr>
<tr>
<td>COV - Modulus [%]</td>
<td>1.78</td>
<td>1.89</td>
</tr>
</tbody>
</table>

Table 2.10. Experimental Comparison of Failure and Damage Theories

<table>
<thead>
<tr>
<th></th>
<th>Macro</th>
<th>Damage/Macro</th>
<th>Damage/Micro/Macro</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min. Difference - Failure Strain [%]</td>
<td>2.89</td>
<td>18.58</td>
<td>7.29</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strain [%]</td>
<td>17.06</td>
<td>33.73</td>
<td>20.13</td>
</tr>
<tr>
<td>Min. Difference - Failure Strength [%]</td>
<td>12.25</td>
<td>15.60</td>
<td>15.53</td>
</tr>
<tr>
<td>Avg. Difference - Failure Strength [%]</td>
<td>12.95</td>
<td>15.67</td>
<td>15.65</td>
</tr>
<tr>
<td>Min. Difference - Modulus [%]</td>
<td>19.81</td>
<td>0.54</td>
<td>~0</td>
</tr>
<tr>
<td>Avg. Difference - Modulus [%]</td>
<td>28.55</td>
<td>12.11</td>
<td>8.06</td>
</tr>
</tbody>
</table>

2.5.4. Impact Simulation Results

Parametric studies were conducted to analyze the failure behavior and residual velocity of the composite plate by varying the $V_f$ of the laminate. For each $V_f$ value, simulations were performed using the same boundary conditions, and were processed using
appropriate time durations that allowed the projectile to penetrate through the composite plate. Stress, strain, and displacement field variables were output for all simulations, as well as the velocity of the projectile at every time step. The tabulated velocity data was plotted and used to compute the residual velocity of the projectile. The velocity of the projectile played a noticeable role in the damage behavior of the impacted composite plate. During an impact event, a portion of the kinetic energy of the projectile was transferred to the composite plate. The simulated damage progression under impact is presented in Figure 2.18 for a projectile traveling at 250 m/s. The geometry was sectioned along a vertical plane to provide a better view of the impact behavior near the projectile/plate interface. As the projectile contacted the plate, the elements on the top surface failed under out-of-plane shear, crushing (compression), and fragmentation. Analysis of the projectile velocity before and after the impact event provides an estimate of the energy absorption of the composite plate under impact.
Figure 2.18. Progression of Projectile Through a Composite Laminate with an Initial Velocity of 250 m/s

Figure 2.19 shows the ballistic limits of composite laminates as a function of $V_f$ where the ballistic limit increases as the $V_f$ increases. The ballistic limit is defined as the velocity required for a projectile to fully penetrate a material specimen and is shown in Equation (2.67) (Jenq, Jing, & Chung, 1994). The parameter $v_p$ represents the velocity of the projectile immediately before impact and $v_r$ is the residual velocity of the projectile after impact.

$$v_{BL} = \sqrt{v_p^2 - v_r^2}$$

Since the density of the fibers is greater than that of the matrix, a larger $V_f$ increases the overall density and stiffness of the composite. Therefore, a greater amount of energy was absorbed by the composite laminates that had higher $V_f$ values. In addition, since the fiber can sustain higher stresses before failure, the composite remained intact for a longer period of time during the impact event; thereby providing more time for the plate to absorb energy from the high speed projectile. A larger number of laminae would absorb more energy, which would cause a greater increase in the ballistic limit.
2.6. Chapter Summary

The sectional micromechanics theory is extended to include material variability through stochastic methodologies, a 3D progressive damage law based on a work potential theory, and a multiscale failure theory. Microstructural characterization of the composite was performed to understand the spatial variability. The integration of the microstructural, statistical data in the sectional micromechanics is achieved using stochastic methodologies, such as general MCS and LHS Monte Carlo simulations. The 3D progressive damage law is used to degrade the elastic properties of the constituents, and the multiscale failure theory is capable of accounting for both subcell and unit cell level failure. For the multiscale impact simulations, the sectional micromechanics with the Hashin failure criteria was
integrated within LS-DYNA. Specifically, the following results and conclusions can be observed:

1. The microstructural characterization results illustrated the spatial variability of the composite material through the bimodal distribution observed for the laminate mosaic, and different distribution functions were determined for the separated microstructure regions.

2. Deterministic results showed that the integration of a multiscale failure criteria and work potential damage theory improved the mechanical behavior and failure response of the composite model.

3. The comparison of the convergence study performed for the stochastic methodologies concluded that the LHS required only 100 simulations, which was approximately 80% fewer simulations than the convergence results using MCS.

4. The quantification of the stochastic results showed that the overall percent difference values of the composite material represented the transverse tensile experimental data better than the deterministic model. The general composite region results showed better correlation with the failure strain of the experiments and the polymer matrix pocket region simulation had a better correlation with the experimental transverse modulus.

5. The developed model is able to simulate the 3D stress-strain states including in-plane shear response and out-of-plane shear response; and the results correlated well with results obtained from the MAC/GMC simulations.
6. The stochastic results from the multiple random variable analysis exhibited the importance of considering the uncertainty in each material parameter since a larger variation in response was observed for an increasing number of random variables.

7. The multiscale impact simulations demonstrated the effect that $V_f$ variability had on the ballistic limit for PMC laminates.
3. **HIGH FIDELITY MICROMECHANICS INCLUDING PROGRESSIVE MATRIX DAMAGE AND THE FIBER/MATRIX INTERPHASE**

3.1. **Introduction**

A major barrier limiting the applications of composites is a lack of confidence in the assessment of safety and reliability of these structures under service conditions. There is a need for accurate predictive tools that take into account constituent interactions, material and architectural variability, and damage at relevant length scales in order to capture the complex damage mechanisms and failure modes. While a significant amount of research has been reported in Chapter 1 which accounts for these length scales and scale bridging, many of these methods assume perfect bonding conditions for the fiber/polymer matrix interphase; whereas the physical structure and interactions at the interphase are not perfect and can be the precursor for damage. The complex interactions between the composite constituents make it difficult to determine damage and predict the failure of these materials. The interphase between composite constituents plays a critical role in the behavior of PMCs and accurate modeling of the interphase is challenging due to the small scale of this region. The focus of this chapter is to apply the progressive damage and multiscale failure theories, detailed in Chapter 2.3, with high fidelity micromechanics to study the effect different fiber/matrix interphase types have on the simulated composite response. High fidelity micromechanics methods consist of higher order displacement fields which allow complex relations between the constituents. A comparison is made by applying interphase properties extracted from several sources (Asp et al., 1996; Wang et al., 2011; B. Zhang et al., 2010). This chapter also presents the details for an interphase model which explicitly
simulates the molecular structure of the region and this model was developed in collaboration with Mr. Bonsung Koo (Johnston, Koo, Subramanian, & Chattopadhyay, 2015).

3.1.1. High Fidelity Generalized Method of Cells Overview

The triply periodic formulation of the HFGMC micromechanical theory is utilized in the current modeling framework and the fundamental equations and description of the HFGMC theory are provided in this chapter for clarity. For the detailed derivation of the HFGMC theory, the reader is directed to Aboudi et al. (2012; 2002). The HFGMC theory extends the MOC (Aboudi 1981; Aboudi 1989; Aboudi 2013) and GMC (Paley & Aboudi, 1992) approaches by incorporating a higher order displacement field to enable complex relations, including shear coupling, between subcells. The composite is considered to have a microstructure consisting of a single fiber in matrix and this is considered the microscale RUC for the material. The RUC is assumed to be periodically distributed in a space defined by the global coordinate system \((x_1, x_2, x_3)\) as illustrated by the leftmost image in Figure 3.1. The RUC geometry is defined within the unit cell coordinate system \((y_1, y_2, y_3)\) with dimensions \(D, H,\) and \(L\). A discretization method is used to divide the unit cell into \(N_\alpha \times N_\beta \times N_\gamma\) subcells. A local subcell coordinate system \((\bar{y}_1^{(\alpha)}, \bar{y}_2^{(\beta)}, \bar{y}_3^{(\gamma)})\) is defined at the center of each subcell with dimensions \(d_\alpha, h_\beta,\) and \(l_\gamma\). The subcells are labeled with the \((\alpha\beta\gamma)\) indices and each subcell may contain a distinct set of material properties. The indexing scheme for the subcells follows the local coordinate system such that \(\alpha = 1, \ldots, N_\alpha\) along the \(y_1\) axis, \(\beta = 1, \ldots, N_\beta\) along the \(y_2\) axis, and \(\gamma = 1, \ldots, N_\gamma\) along the \(y_3\) axis. It is also important to note that in this theory the \((\alpha\beta\gamma)\) indices do not indicate summation.
3.1.1.1. Governing Equations

The 3D equilibrium equations for a subcell \((\alpha\beta\gamma)\) are defined by

\[
\frac{\partial}{\partial y_1^{(\alpha)}} \sigma_{i1}^{(\alpha\beta\gamma)} + \frac{\partial}{\partial y_2^{(\beta)}} \sigma_{i2}^{(\alpha\beta\gamma)} + \frac{\partial}{\partial y_3^{(\gamma)}} \sigma_{i3}^{(\alpha\beta\gamma)} = 0, \quad i = 1, 2, 3 \tag{3.1}
\]

where \(\sigma^{(\alpha\beta\gamma)}\) represents the stress components for the subcell \((\alpha\beta\gamma)\). Using a volume averaging derivation method, the averaged form of Equation (3.1), in terms of surface average tractions, \(t_i\), is presented as

\[
\frac{1}{d_x} \left( \tau_i^{(1)+} - \tau_i^{(1)-} \right) + \frac{1}{h_y} \left( \tau_i^{(2)+} - \tau_i^{(2)-} \right) + \frac{1}{l_z} \left( \tau_i^{(3)+} - \tau_i^{(3)-} \right) = 0 \tag{3.2}
\]

where the left superscript numeral of the tractions represents the normal direction of the surfaces being averaged over. Since two surfaces are present for each direction, a superscript with a positive or negative symbol is used to represent the specific surface at the positive or negative position along that direction. The expressions for the surface average tractions are given in Equations (3.3)-(3.5) where the integration is performed using half the subcell dimensions since the local subcell coordinate system is defined at the...
center of the subcells. Additionally, the stress components are presented as functions of displacement variables which will be detailed in later sections of this chapter.

\[
(1) \quad t_{i}^{(a\beta\gamma)} = \frac{1}{h_{\beta}\gamma} \int_{-h_{\beta}/2}^{h_{\beta}/2} \int_{-l_{i}/2}^{l_{i}/2} \sigma_{i}^{(a\beta\gamma)} \left( \tilde{y}_{i}^{(a)} = \pm \frac{d_{a}}{2} \right) d\tilde{y}_{3}^{(\gamma)} d\tilde{y}_{2}^{(\beta)}
\]

\[
(2) \quad t_{i}^{(a\beta\gamma)} = \frac{1}{d_{\alpha}\gamma} \int_{-d_{\alpha}/2}^{d_{\alpha}/2} \int_{-l_{i}/2}^{l_{i}/2} \sigma_{2i}^{(a\beta\gamma)} \left( \tilde{y}_{i}^{(\beta)} = \pm \frac{h_{\beta}}{2} \right) d\tilde{y}_{3}^{(\gamma)} d\tilde{y}_{i}^{(a)}
\]

\[
(3) \quad t_{i}^{(a\beta\gamma)} = \frac{1}{d_{\alpha}h_{\beta}} \int_{-d_{\alpha}/2}^{d_{\alpha}/2} \int_{-h_{\beta}/2}^{h_{\beta}/2} \sigma_{3i}^{(a\beta\gamma)} \left( \tilde{y}_{3}^{(\gamma)} = \pm \frac{l_{\gamma}}{2} \right) d\tilde{y}_{2}^{(\beta)} d\tilde{y}_{i}^{(a)}
\]

3.1.1.2. Higher Order Displacement Field

The basis for the HFGMC theory is the second order expansion of the displacements, \( u_{i}^{(a\beta\gamma)} \), defined in Equation (3.6) for a subcell \((a\beta\gamma)\).

\[
u_{i}^{(a\beta\gamma)} = \bar{\varepsilon}_{ij} x_{j} + W_{i}^{(a\beta\gamma)} + \tilde{y}_{1}^{(a)} W_{i}^{(a\beta\gamma)} + \tilde{y}_{2}^{(\beta)} W_{i}^{(a\beta\gamma)} + \tilde{y}_{3}^{(\gamma)} W_{i}^{(a\beta\gamma)} + \frac{1}{2} \left( 3\tilde{y}_{1}^{(a)2} - \frac{d_{a}^{2}}{4} \right) W_{i}^{(a\beta\gamma)} + \frac{1}{2} \left( 3\tilde{y}_{2}^{(\beta)2} - \frac{h_{\beta}^{2}}{4} \right) W_{i}^{(a\beta\gamma)} + \frac{1}{2} \left( 3\tilde{y}_{3}^{(\gamma)2} - \frac{l_{\gamma}^{2}}{4} \right) W_{i}^{(a\beta\gamma)}
\]  

The \( \bar{\varepsilon}_{ij} \) tensor contains the average global strain components applied to the RUC and \( W_{i}^{(a\beta\gamma)} \) are the volume averaged displacements. The remaining \( W_{i}^{(a\beta\gamma)} \) are higher order terms where \( l, m, \) and \( n \) may equal 0, 1, or 2.
3.1.1.3. Boundary and Interfacial Conditions

The volume averaged displacements $W_{i(000)}^{(\alpha\beta\gamma)}$ and higher order terms $W_{i(lmn)}^{(\alpha\beta\gamma)}$ are solved through the application of appropriate constitutive laws, governing equations, subcell interfacial conditions, and periodic RUC boundary conditions. The exact forms of the periodic boundary conditions for the displacement field of the RUC are represented by

$$u_i\left(y_1 = 0\right) = u_i\left(y_1 = D\right) \quad (3.7)$$

$$u_i\left(y_2 = 0\right) = u_i\left(y_2 = H\right) \quad (3.8)$$

$$u_i\left(y_3 = 0\right) = u_i\left(y_3 = L\right) \quad (3.9)$$

and the exact forms of the periodic stress boundary conditions are given by

$$\sigma_{ii}\left(y_1 = 0\right) = \sigma_{ii}\left(y_1 = D\right) \quad (3.10)$$

$$\sigma_{2i}\left(y_2 = 0\right) = \sigma_{2i}\left(y_2 = H\right) \quad (3.11)$$

$$\sigma_{3i}\left(y_3 = 0\right) = \sigma_{3i}\left(y_3 = L\right) \quad (3.12)$$

In the HFGMC theory, the averaged forms of the displacement periodic boundary conditions, from Equations (3.7)-(3.9), are expressed by the following

$$\int_{-h/2}^{h/2} \int_{-l/2}^{l/2} u_i^{(\alpha\beta\gamma)} \left(\tilde{y}_1^{(i)} = -\frac{d_1}{2}\right) d\tilde{y}_1^{(\gamma)} d\tilde{y}_2^{(\beta)} = \int_{-h/2}^{h/2} \int_{-l/2}^{l/2} u_i^{(\alpha\beta\gamma)} \left(\tilde{y}_1^{(N_{\alpha\beta\gamma})} = \frac{d_{N_{\alpha\beta\gamma}}}{2}\right) d\tilde{y}_1^{(\gamma)} d\tilde{y}_2^{(\beta)} \quad (3.13)$$

$$\int_{-d/2}^{d/2} \int_{-l/2}^{l/2} u_i^{(\alpha\gamma\lambda)} \left(\tilde{y}_2^{(i)} = -\frac{h}{2}\right) d\tilde{y}_3^{(\gamma)} d\tilde{y}_1^{(\alpha)} = \int_{-d/2}^{d/2} \int_{-l/2}^{l/2} u_i^{(\alpha\gamma\lambda)} \left(\tilde{y}_2^{(N_{\alpha\gamma\lambda})} = \frac{h_{N_{\alpha\gamma\lambda}}}{2}\right) d\tilde{y}_3^{(\gamma)} d\tilde{y}_1^{(\alpha)} \quad (3.14)$$
Similarly, the averaged forms of the stress periodic boundary conditions, from Equations (3.10)-(3.12), are as follows.

\[
\begin{align*}
(1) & \quad I_i^{(-1\beta\gamma)} = I_i^{+(N\alpha\beta\gamma)} \\
(2) & \quad I_i^{(-\alpha1\gamma)} = I_i^{+(\alpha N\beta\gamma)} \\
(3) & \quad I_i^{(-\alpha\beta1)} = I_i^{+(\alpha N\gamma)}
\end{align*}
\]  

(3.16)  

(3.17)  

(3.18)

Assuming perfect continuity for the subcell interface, the continuous displacement expressions, comparable to the periodic boundary relationships, can be established as described in Equations (3.19)-(3.21).

\[
\begin{align*}
\int_{-h/2}^{h/2} \int_{-l/2}^{l/2} u_i^{(\alpha\beta\gamma)} \left( y_3^{(\alpha)} = \frac{d_{\alpha}}{2} \right) dy_3^{(\alpha)} dy_2^{(\beta)} &= \int_{-h/2}^{h/2} \int_{-l/2}^{l/2} u_i^{(\alpha+1\beta\gamma)} \left( y_3^{(\alpha+1)} = -\frac{d_{\alpha+1}}{2} \right) dy_3^{(\alpha+1)} dy_2^{(\beta)} \\
\int_{-d/2}^{d/2} \int_{-l/2}^{l/2} u_i^{(\alpha\beta\gamma)} \left( y_2^{(\beta)} = \frac{h_{\beta}}{2} \right) dy_3^{(\alpha)} dy_2^{(\beta)} &= \int_{-d/2}^{d/2} \int_{-l/2}^{l/2} u_i^{(\alpha\beta+1\gamma)} \left( y_2^{(\beta+1)} = -\frac{h_{\beta+1}}{2} \right) dy_3^{(\alpha)} dy_2^{(\beta)} \\
\int_{-d/2}^{d/2} \int_{-h/2}^{h/2} u_i^{(\alpha\beta\gamma)} \left( y_3^{(\gamma)} = \frac{l_{\gamma}}{2} \right) dy_2^{(\beta)} dy_1^{(\alpha)} &= \int_{-d/2}^{d/2} \int_{-h/2}^{h/2} u_i^{(\alpha\beta\gamma+1)} \left( y_3^{(\gamma+1)} = \frac{l_{\gamma+1}}{2} \right) dy_2^{(\beta)} dy_1^{(\alpha)}
\end{align*}
\]  

(3.19)  

(3.20)  

(3.21)

Additionally, the continuity of tractions between adjoining subcells can be defined by expressions, similar to the periodic boundary conditions, presented in Equations (3.22)-(3.24). It is important to note that these stress and displacement continuity conditions at the subcell interfaces are only valid if the \((\alpha+1), (\beta+1),\) and \((\gamma+1)\) index values in the right hand side of the equations are less than or equal to \(N_\alpha, N_\beta,\) and \(N_\gamma,\) respectively.
Simplified expressions are obtained by defining the governing equations, periodic boundary conditions, and subcell interfacial conditions in terms of the volume averaged displacements $W_{i(000)}^{(a\beta\gamma)}$ and higher order terms $W_{i(0mn)}^{(a\beta\gamma)}$. The simplified equations are compiled into a system of equations and matrix operations are applied to obtain a solution and the detailed solution procedure is provided in Aboudi et al. (2012, 2002). The solved values for the volume averaged displacement and higher order terms are used and the average stress in the composite RUC is calculated using

$$\bar{\sigma}^{(RUC)} = \frac{1}{DHL} \sum_{\alpha=1}^{N_\alpha} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} d_{\alpha} h_{\beta} l_{\gamma} \bar{\sigma}^{(a\beta\gamma)}$$

(3.25)

where $\bar{\sigma}^{(a\beta\gamma)}$ is the volume averaged stress of the subcell determined through Equation (3.26).

$$\bar{\sigma}^{(a\beta\gamma)} = \frac{1}{d_{a} h_{\beta} l_{\gamma}} \int_{-h_{\beta}/2}^{h_{\beta}/2} \int_{-l_{\gamma}/2}^{l_{\gamma}/2} \int_{-d_{a}/2}^{d_{a}/2} \sigma^{(a\beta\gamma)} dy_3 dy_2 dy_1$$

(3.26)

### 3.2. Implementation of HFGMC with the Fiber/Matrix Interphase

#### 3.2.1. Microscale with Interphase

Since the composite unit cell is defined by a continuous carbon fiber, the computational costs of the microscale simulations are reduced by setting the unit cell thickness in the $y_j$ direction to be one subcell thick. The interphase subcells are created by
replacing the polymer subcells that are immediately adjacent to the fiber subcells as illustrated in Figure 3.2. A unit cell discretized into 256 subcells is shown as an example, and a convergence study in the results section of this chapter is used to determine the appropriate number of subcells needed to represent the unit cell. The properties of the interphase are incorporated into the HFGMC micromechanics approach to obtain the unit cell response of the composite.

3.2.2. Constitutive Laws

The remaining expressions needed to solve the system of equations for the HFGMC theory are the constitutive laws for the subcells. The material systems for the fiber and polymer matrix constituents are defined as transversely isotropic linear elastic and isotropic viscoplastic materials, respectively. A single digit index is computed from the three digit,
Greek character index of the original HFGMC theory in order to develop the code using vectors for the geometric and material parameters. The single digit index converts the three digit code using

\[ subind = N_\beta N_\gamma (\alpha - 1) + N_\gamma (\beta - 1) + \gamma \]  

(3.27)

where \( subind \) replaces the three digit index code, \((\alpha\beta\gamma)\), and a 2D slice showing an arbitrary unit cell cross-section is presented in Figure 3.3 to compare the two index codes.

![Figure 3.3](image)

Figure 3.3. Indexing of the Subcells using (a) a Three Digit Code and (b) a Single Digit Code

The constitutive equations for the fiber and polymer subcells are shown in Equation (3.28) and Equation (3.29), respectively.

\[ \sigma_{ij}^{(subind)} = C_{ijkl}^{(subind)} \varepsilon_{ij}^{(subind)} \quad i, j, k, l = 1, 2, 3 \]  

(3.28)

\[ \sigma_{ij}^{(subind)} = C_{ijkl}^{(subind)} (\varepsilon_{ij}^{(subind)} - \varepsilon_{ij}^{(subind)}) \quad i, j, k, l = 1, 2, 3 \]  

(3.29)

The total strains of the subcells are given by

\[ \varepsilon_{ij}^{(subind)} = \frac{1}{2} \left( \partial_j u_i^{(subind)} + \partial_i u_j^{(subind)} \right) \quad \partial_i, \partial_j = \frac{\partial}{\partial y_1^{(\alpha)}}, \frac{\partial}{\partial y_2^{(\beta)}}, \text{ or } \frac{\partial}{\partial y_3^{(\gamma)}} \]  

(3.30)
The inelastic strains, $\varepsilon^{I_{\text{subind}}}$, are determined using the modified Bodner-Partom viscoplastic theory and inelastic properties outlined in Chapter 2.3.3. The 3D properties for the fiber and polymer are also presented in the previous chapter (Table 2.3 and Table 2.4). For computational efficiency, a column vector containing the constituent phase for each subcell is defined where each constituent material type is represented by a unique number. Hence, the material properties and stiffness matrices of the constituent materials only need to be defined once and the phase vector will be used to determine which stiffness matrix is applied to each subcell. The polymer subcells use a stiffness matrix as described, using Voigt notation, in Equation (3.31) where $p_d$ is the damage parameter for the elastic modulus which is determined by the previously detailed 3D damage theory in Chapter 2.3.2. Each polymer subcell has an individual $p_d$ parameter which is used to degrade the stiffness matrix only for the corresponding matrix subcell.

$$
C^{(\text{subind})} = \frac{P^{(\text{subind})}_{d}E_{m}}{(1+\nu)(1-2\nu)} \begin{bmatrix}
1-\nu & \nu & \nu & 0 & 0 & 0 \\
\nu & 1-\nu & \nu & 0 & 0 & 0 \\
\nu & \nu & 1-\nu & 0 & 0 & 0 \\
0 & 0 & 0 & (1-2\nu)/2 & 0 & 0 \\
0 & 0 & 0 & 0 & (1-2\nu)/2 & 0 \\
0 & 0 & 0 & 0 & 0 & (1-2\nu)/2 \\
\end{bmatrix}
$$

In order to compare with different interphase properties from literature, the constitutive law for the interphase subcells is assumed to be linear elastic with either isotropic or transversely isotropic material orientations. The multiscale failure theory from Chapter 2.3.4 is used for the unit cell response in order to capture micro- and macroscale failure modes. A maximum stress criterion is utilized for the microscale failure of the interphase subcells and the failure strengths of the interphase are presented later in Table 3.1. A maximum strain criterion is employed for the polymer subcells due to the highly nonlinear...
response caused by the viscoplastic nature of the polymer. The macroscale failure criteria of the unit cell are based on a modified Hashin failure theory.

3.2.3. Interphase Types and Properties

This subsection presents the development of an interphase model, in collaboration with Mr. Bonsung Koo, which explicitly simulates the molecular structure of the interphase; and further details of the nanoscale model and results are presented by Johnston et al. (2015). The molecular interphase model replicates the semi-crystalline structure of the carbon fiber surface by intentionally creating voids in several protruded graphene layers. The carbon fiber surface model is constructed by stacking a number of pristine graphene layers and the graphene layers with the void. The combination of the carbon fiber surface and polymer matrix constituents for the molecular interphase model are depicted in Figure 3.4. The numerical curing of the resin and hardener allows the polymer network to form through the void of the graphene layer, capturing entanglement between the carbon fiber surface and the polymer matrix. Due to this entanglement of polymer chains, a large amount of energy is required to break these bonds compared to the non-bonded interactions between the constituents. The initial dimensions of the interphase model are 100×65×50 Å³, and the model consists of 15,000 atoms in the polymer matrix and 15,840 atoms in the carbon fiber surface. The virtual testing using the interphase model are conducted to obtain the molecular generated properties of the interphase, which are then used in the constitutive laws of the interphase subcells defined by the high fidelity micromechanics theory.
Additionally, various interphase properties from literature are applied to investigate the transverse tensile response obtained by the micromechanical simulations. Table 3.1 displays the transverse properties for each interphase type including the molecular interphase model. The interphase properties utilized by Wang et al. (2011) were obtained using dynamic modulus imaging methods. Zhang et al. (2010) calculated the interphase properties using a cohesive law derived from the Lennard-Jones potential and they applied factors to capture microscopic defects. A parametric study was performed by Asp et al. (1996) to study the sensitivity of assumed interphase properties on larger length scales.
Table 3.1. Interphase Material Properties

<table>
<thead>
<tr>
<th></th>
<th>Transverse Modulus (GPa)</th>
<th>Transverse Tensile Strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wang et al. (2011)</td>
<td>12.7</td>
<td>50</td>
</tr>
<tr>
<td>Zhang et al. (2010)</td>
<td>3.37</td>
<td>53</td>
</tr>
<tr>
<td>Asp et al. (1996)</td>
<td>34</td>
<td>50*</td>
</tr>
<tr>
<td>Johnston et al. (2015)</td>
<td>8.28</td>
<td>1024</td>
</tr>
</tbody>
</table>

* Value assumed; not available in reference

3.3. Results and Discussion

3.3.1. Convergence Study

An initial convergence study was performed to determine an appropriate time step and a sufficient number of subcells required for the micromechanics simulations. The developed molecular interphase model was applied for this convergence study. The transverse tensile modeling results are obtained by applying a strain rate of 1.05 s\(^{-1}\) to the PMC microscale unit cell. The unit cell stress-strain response for various time steps are plotted for the results with only viscoplasticity (Figure 3.5a) and the results with the added damage and failure theories (Figure 3.5b). This study demonstrated that by adding complexities to the model, such as the damage and failure theories, the convergence required a smaller time step. Overall, convergence is achieved with a time step of 5E-6 seconds. It is important to note that, for the time step convergence, a unit cell geometry with 64 subcells is used to ensure that the converged time step will be applicable for unit cells with more subcells. The convergence study for the number of microscale subcells is presented in Figure 3.6 and shows that the unit cell stress-strain response converges with a
simulation containing 256 subcells. The converged parameters are used in the subsequent simulations to compare the different interphase models and properties.

Figure 3.5. Convergence Study of the Time Step for Simulation Results (a) with Viscoplasticity and (b) with the Added Damage and Failure Theories

Figure 3.6. Convergence Study of the Number of Subcells using the Modeling Framework with the Damage and Failure Theories
3.3.2. Comparison of Different Interphase Models

Transverse tensile stress-strain plots of unit cell simulations with different interphase types are depicted in Figure 3.7. The top plot in the figure portrays the responses from the modeling framework applying only the elastic and viscoplastic laws; whereas, the bottom plot shows the simulation results obtained by adding the damage and multiscale failure criteria. For comparison, these results are plotted with responses obtained from a unit cell geometry without interphase subcells (illustrated in Figure 3.2a); and these responses are indicated as “None” in the plot legends. The stress-strain response for the simulations with interphase properties from literature (Table 3.1) shows smaller failure strains compared to the simulation without interphase subcells. In contrast, the simulations with the molecular interphase model result in a 5% lower transverse tensile strength and increased nonlinearity causing 25% larger failure strains. The difference between the top and bottom plots is minimal in the elastic region but, after the yield point, an increase in nonlinearity is shown for the stress-strain responses with the added damage and failure theories. This phenomenon is highlighted by the large, dotted red line in the figure where the arrows of the line emphasize the fact that the stress, for a strain value of 0.7%, is lower for the results with the added damage and failure theories. However, additional analysis of the results is needed to determine the local causes of damage and failure.
Figure 3.7. Simulated Transverse (22) Tension Stress-Strain Plots Comparing Different Interphase Properties in the Model with Elasticity and Viscoplasticity (Top), and Adding Damage and Failure Theories (Bottom)

Plotting the stress and strain distributions from the subcells provides the local information needed to study the effect of the different interphase properties on viscoplasticity and damage. To plot the transverse strain as a function of normalized unit cell width, subcell strain values are extracted as shown by the arrow bisecting the unit cell in the $y_2$ direction in Figure 3.2. Figure 3.8 contains a series of subcell strain-width plots for progressively increasing unit cell strains. The plots on the left of the figure are obtained
from results only applying the elastic and viscoplastic laws and the plots on the right demonstrate the results with the added microdamage and multiscale failure criteria. For the strain-width distributions extracted from the elastic region (Figure 3.8a and b), the response shows small strain gradients forming at the interphase for each type of interphase which exhibits the difference in stiffness between the composite constituents and indicates that the type of interphase has minimal effect on the strain distribution in the elastic regime. For unit cell strains past the elastic regime, the strain concentrations at the ends of the unit cell grow substantially for the simulations with the molecular interphase model. Furthermore, the trends between the left and right strain-width plots are identical except at the interphase where the results with the damage and failure theories yield larger strain gradients. These outcomes indicate that the material properties at the interphase become more compliant due to local damage and failure.

(a) 0.15% Unit Cell Strain

(b) 0.15% Unit Cell Strain
Figure 3.8. Strain-Width Distributions for Simulated Behavior with Viscoplasticity (a,c, and e) and Behavior with Viscoplasticity Plus Damage and Failure (b,d, and f)

Figure 3.9 presents the subcell stress-width distributions for different unit cell strains. For the elastic regime, the stress-width plots show minimal variation for different interphase types, which is similar in trend to the strain-width plots. However, stress
concentrations exist at the ends of the unit cell and, contrary to the strain-width data, the stress-width results from the elastic regime illustrate a large stress gradient for the simulations with the molecular interphase model. For a unit cell strain of 0.74%, the subcell stress-width data for the simulations with the literature interphase types indicates local failure of the interphase subcells. In contrast, local failure occurs in the polymer subcells for the unit cell simulations with the molecular interphase model. Additionally, the simulations with the molecular interphase model show that the stress gradient at the interphase grows with increasing unit cell strain due to the properties and material symmetry applied to these models. Moreover, for large unit cells strains, the results with the molecular interphase model deviate in the middle of the plots which implies that the molecular interphase affects the behavior in the fiber subcells as well. It is important to note that the large variations in transverse elastic moduli of different interphase types does not affect the mode of local failure, whereas the interphase strength and structure does affect the mode of local failure.

Similar conclusions about failure were made by Maligno et al. (2010) where a FEA model of a composite RVE was simulated and parametric studies were performed using interphase strength as a variable. For interphase strengths less than 60 MPa, Maligno’s results showed that local failure initiated in the interphase elements and, for higher values of interphase strengths, local failure occurred in the polymer elements. These results were obtained using varying interphase transverse elastic moduli and the moduli variations did not have an effect on the mode of local failure which agrees with the results from the current simulations.
Figure 3.9. Stress-Width Distributions for Simulated Behavior with Viscoelasticity (a and c) and Behavior with Viscoelasticity Plus Damage and Failure (b and d)

3.4. Chapter Summary

A modeling framework was used to integrate progressive damage, multiscale failure, and interphase properties within an HFGMC micromechanics theory. Micromechanics
simulations were performed to investigate the effect of the interphase on the behavior obtained by the model. The molecular interphase model detailed in this chapter is composed of multiple graphene layers with voids and a thermoset polymer matrix to represent the physical molecular structure of the interphase. The graphene layers with voids layers were created by removing carbon atoms which caused voids in the layers. For comparison, the interphase properties extracted from the literature were incorporated within the current modeling framework. The usage of this modeling framework yielded the following results and observations:

1. The transverse tensile results showed that the unit cell response, with the developed molecular interphase model, predicted a composite tensile strength that was approximately 5% lower than the other interphase types and also predicted a maximum difference of 25% in failure strain.

2. A convergence study was performed by varying the time step and the number of subcells for a unit cell simulation, and the results demonstrate that a time step of 5E-6 seconds and a unit cell with 256 subcells are required for convergence.

3. The strain-width distributions demonstrate, for unit cell strains past the elastic regime, large strain concentrations at the ends of the unit cell for the simulations with the molecular interphase model, and the results with the damage and failure theories yield larger strain gradients and damage at the interphase.

4. The stress-width plots show large strain gradients forming at the interphase and ultimately leading to local interphase failure, for the literature interphase types, and polymer failure for the molecular interphase model.

5. Additionally, for large unit cell strains, the stress-width results for the molecular
interphase deviate in the middle of the plots suggesting that the molecular interphase model significantly impacts the behavior in the fiber subcells as well.
4. EFFECT OF ENVIRONMENTAL CONDITIONS ON THE MECHANICAL PROPERTIES AND DAMAGE OF TRIAXIAL BRAIDED COMPOSITES

4.1. Introduction

In regards to aerospace applications, there is interest in using braided composite architectures because of their advantageous characteristics such as delamination prevention. However, as mentioned in Chapter 1, limited studies on braided composites hinder the application of these materials. Additionally, aerospace structures experience extreme environmental conditions, and reliability analyses need to consider these effects. This chapter discusses the effects of environmental conditioning on the tensile, compressive, and in-plane shear properties of triaxial braided PMCs, which were tested under room, hot (100°C), and hot/wet conditions (60°C/90% relative humidity). A humidity and temperature controlled chamber was used for the hot/wet conditioned specimens. A volume fraction study was performed to obtain a statistical range for the volume fraction parameters from multiple manufactured panels. A DIC system was used with a mechanical test frame to obtain the full field strain on the surface of the specimens and to examine strain at the edges of the specimens. A flash thermography technique was used to examine structural degradation on the surface and sub-surface at the center and edges of each specimen, and scanning electron microscopy was performed to study the effects of environmental conditions on the damage mechanisms.
4.2. Experimental Methods

4.2.1. Material Specifications

In this chapter, a six-layer laminate of triaxial braided composite material is used, having a total thickness of 3.175 mm (0.125 in.). The material consists of CYCOM PR-520 epoxy resin (Cytec Industries, Inc.) and high strength, standard modulus TORAY T700S carbon fibers (Toray Carbon Fibers America, Inc.). The constituent properties, as reported by the manufacturers, are presented in Table 4.1. North Coast Composites manufactured the composite panels using a resin transfer molding (RTM) technique and specimens were machined from these panels. A $0^\circ/ +60^\circ/ -60^\circ$ triaxial braid architecture was used and the top view of the RUC is defined by the outlined box and dimensions in Figure 4.1. An RUC is defined as the smallest repeating volume of geometry that can represent the composite material. The blue vertical arrow in the figure indicates the direction of the axial fiber tows (24,000 fibers per tow) and the other white arrows indicate the bias braid tows (12,000 fibers per tow) oriented in the $\pm 60^\circ$ directions.

<table>
<thead>
<tr>
<th>Table 4.1. Constituent Material Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resin/Fiber</td>
</tr>
<tr>
<td>----------------------</td>
</tr>
<tr>
<td>T700S fibers</td>
</tr>
<tr>
<td>PR-520 resin</td>
</tr>
</tbody>
</table>
The volume fractions of the constituents in the triaxial composite material were measured following the American Society for Testing and Materials (ASTM) D3171 (2006) standard, and the experiments were performed using the resin burn-off technique detailed in Procedure G of the standard. Samples were extracted from multiple locations in several of the manufactured composite panels in order to obtain a statistical range of volume fraction values and to compare the difference in volume fraction data between the panels. The dimensions of the volume fraction samples were 2.5 cm by 2.5 cm (1 in. by 1 in.) with a thickness of 3.175 mm (0.125 in.) and were dried in a thermal chamber at a standard temperature of 90°C. The mass of each sample, before experimentation, was approximately 5 grams, which complies with the minimum recommended mass of 1 gram defined in the standard. As shown in Figure 4.2(a), samples were placed in a metal crucible before testing in order to contain all the remnant material for weight measurements and to prevent particle and oil contamination on the samples. The resin burn-off procedure was performed by placing the samples in an Isotemp 550 (Fisher Scientific) muffle furnace at 550°C. After 6 hours in the muffle furnace, the weight of the remnant carbon fiber (Figure 4.2b) from each sample was measured.
A total of sixteen samples were tested for the volume fraction experiment and the data for each sample is included in Table 4.2. The table includes measurements of the specimen mass which was made before the experiment; the mass of the carbon fiber was weighed after the resin was burned off. The mass of the resin was calculated by subtracting the carbon fiber mass from the initial specimen mass measurements. The fiber volume fraction \((V_f)\) and matrix volume fraction \((V_m)\) were calculated using Equation (4.1) and Equation (4.2), respectively. The void volume fraction \((V_v)\) was calculated from the fiber and matrix volume fraction as described by Equation (4.3). The average volume fractions of all sixteen specimens are presented at the bottom of Table 4.2.

\[
V_f[\%] = \frac{M_f}{M_i} \times \frac{\rho_c}{\rho_f} \times 100
\]  

(4.1)

\[
V_m[\%] = \frac{(M_i - M_f)}{M_i} \times \frac{\rho_c}{\rho_m} \times 100
\]  

(4.2)

\[
V_v[\%] = 100 - V_f - V_m
\]  

(4.3)

In Equations (4.1) and (4.2), \(M_i\) represents the mass of the specimen before the experiment and \(M_f\) is the mass of the fibers after the resin was burned off. The composite density \((\rho_c)\) of each sample was computed by using the volume measured from the average length, width, and height values of each sample as well as the sample’s mass (Table 4.2). The manufacturer values for the carbon fiber density \((\rho_f)\) and the resin matrix density \((\rho_m)\) are provided in Table 4.1.
(a) Before Resin Burn-Off Test  
(b) After Resin Burn-Off Test

Figure 4.2. Images of a Triaxial Composite Volume Fraction Sample (a) Before and (b) After a Resin Burn-Off Test

Table 4.2. Volume Fraction Data

<table>
<thead>
<tr>
<th>Sample</th>
<th>Panel</th>
<th>Sample Mass (g.)</th>
<th>Sample Density (g/cm³)</th>
<th>Fiber Mass (g.)</th>
<th>Resin Mass (g.)</th>
<th>Vf (%)</th>
<th>Vm (%)</th>
<th>Vv (%)</th>
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<td>2.2289</td>
<td>52.53</td>
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Mean: 52.59 46.79 0.619
4.2.2. Specimen Geometries

Specimens were designed to obtain the tensile, compressive, and shear properties for the triaxial braided composite material. The ASTM standards (D3410, 2003; D3039, 2003; D7078, 2004) were used to guide the design of the compression, tension, and shear specimens. The averaged dimensions for the specimen geometries are displayed in Figure 4.3. Tension and compression tests were performed for both axial (parallel to the 0° axial tows) and transverse (perpendicular to the 0° axial tows) directions. However, results from previous studies (Kohlman et al., 2012; Littell et al., 2009; Roberts et al., 2009) have shown that the ASTM D3039 geometry yields premature damage and lower strength in transverse tension specimens due to the large size of the RUC and specimen edge effects. Notched (Kohlman et al., 2012) and bowtie (Bowman, Roberts, Braley, Xie, & Booker, 2003) specimens have been tested in past studies in order to improve the transverse tensile results. Although higher strengths were noted for the notched geometry, the specimen contained a non-uniform gage region which resulted in a sharp stress concentration. In the current work, a version of the bowtie geometry presented by Bowman et al. (2003) was used to examine the transverse tension response and edge effects.
Figure 4.3. Average Dimensions of the Geometries for (a) Transverse Bowtie, (b) Compression, (c) Tension, and (d) V-Notched Rail Shear Specimens

4.2.3. Mechanical Testing Equipment

The specimens were tested using an Instron 5985 mechanical test frame in displacement control at a constant rate of 0.635 mm/min (0.025 in/min). A two-camera DIC system (GOM ARAMIS 2M) was time synchronized with the test frame to study the strain field of the specimen through non-contact measurements. The DIC software uses pattern recognition algorithms to calculate deformation and strain at each stage by correlating the data with a reference stage (GOM, 2006). An airbrush was used to paint a white background on the surface of each specimen and a black speckle pattern was applied to this background in order for the DIC system to compute the strain field on the specimen surface. Before testing, calibration of the DIC was performed using a set of calibration
panels, which were specified based on the current camera setup and field of view needed for the specimen. A selected area of the processed strain field (Figure 4.4), with approximately 250 data points, was used to calculate the average global strain. For each specimen geometry, the global strain measure was selected at an area away from the edges of the specimen to reduce the effect of strain concentrations on this measure.

![Selected Area of an Axial Tensile Strain Field](image)

Figure 4.4. Selected Area of an Axial Tensile Strain Field

In order to facilitate the specimen testing, several fixtures were used on the mechanical frame. For tension and bowtie specimens, testing was performed using hydraulic grips equipped on the test frame. The v-notched rail shear fixture (Wyoming Test Fixtures, Inc.), shown in Figure 4.5, was installed for the testing of the in-plane shear specimens. It uses a set of bolts and surfalloy coated grips to apply gripping pressure to the surface of the specimen. The design of an ASTM D3410 fixture (shown in Figure 4.6) was modified in
order to accommodate the DIC strain measurement system for compression testing. Adapters were modified to connect the compression fixture to the test frame and to reduce the width and overall length of the fixture setup; thereby ensuring that the fixture fit properly inside the environmental chamber. Compression specimens were gripped by lateral pressure applied through the tapered slots, and end loading was provided by wedges placed underneath the grips inside the fixture. The grip halves were threaded, and bolts (shown in Figure 4.6b) were used for alignment and to apply initial pressure on the surface of the specimen to prevent slipping during the test.

Figure 4.5. ASTM D7078 V-Notched Rail Shear Test Fixture
A nondestructive, pulsed flash thermography technique was performed to determine intrinsic flaws and damage on the surface and sub-surface of the specimens. The flash thermography technique was performed using an EchoTherm system (Thermal Wave Imaging, Inc.) with an InSb infrared focal plane array camera operating at 60 Hz. The surface of the specimen was exposed to heat through a short pulse of light from a set of flash lamps. The infrared camera was used to capture the temperature field of the specimen during and after the flash pulse for a predetermined period of time. A Hitachi S-4700 scanning electron microscope, set at a low voltage (1-2 kV), was used to examine the modes of failure at different stress levels. This low voltage setting was applied to prevent damage on the surface of the specimen.
4.3. Environmental Conditioning

The following environmental conditions were applied to the triaxial braided specimens: i) room condition (baseline comparison), ii) hot condition (100°C), and iii) hot/wet condition (60°C/90% relative humidity). A removable thermal chamber on the mechanical frame was used for simultaneous heating and testing for the hot condition. Specimens were placed in the removable thermal chamber for 15 minutes before being gripped and tested. For the hot/wet condition, specimens were placed in an environmental chamber with the aforementioned temperature and humidity parameters. The weight of the specimens was measured periodically throughout the environmental conditioning process to assess the amount of moisture absorption. The data shows that after 12 weeks the weight gain due to moisture absorption converged to 0.45% (Figure 4.7). Periodic weighing procedures and convergence metrics, outlined in the ASTM D5229 (2004a), were followed for this conditioning process. After conditioning, hot/wet specimens were removed from the environmental chamber and mechanically tested at 100°C.
4.4. Results and Discussion

4.4.1. Tensile Response

A minimum of five specimens were tested for each type of test. The stress-strain plots for each of the transverse and axial tension specimens are presented in Figure 4.8 and Figure 4.9, respectively. The axial tensile response is almost linear for all the specimens, but nonlinear behavior was observed in the transverse direction. The braid angle and lack of tow continuity between the top and bottom grip surfaces in the transverse tension specimen are potential causes for the nonlinear behavior as well as the lower elastic modulus and transverse strength. The edge effects located at the bias braid termination points in the transverse tension specimens cause premature damage such as subsurface axial tow splitting. For the transverse tensile response, the environmental conditions caused reductions in the Proportional Elastic Limit (PEL) indicating that macroscopic damage occurred at lower strains. The reductions in PEL strains as well as the mean and standard deviation for the elastic and failure properties of the tensile tests are shown in Table 4.3. A possible reason for the lower PEL strains and increased nonlinearity in the transverse results is earlier axial tow splitting and this phenomenon is quantified later in this chapter. The mechanical properties for the room condition correlate well with properties and trends presented in previous studies (Kohlman et al., 2012; Littell et al., 2009; Roberts et al., 2009). Unlike the transverse tension direction, the axial tension results show that the environmental conditions affect the failure strength and Poisson’s ratio with minimal effect on the elastic modulus. No significant difference was observed between the hot and hot/wet conditions.
Figure 4.8. Stress-Strain Plots for Each Transverse Tensile Specimen (PEL Strains are Indicated by Red Triangles)

Figure 4.9. Stress-Strain Plots for Each Axial Tensile Specimen
<table>
<thead>
<tr>
<th>Condition</th>
<th>Material Parameter</th>
<th>Failure Stress [MPa]</th>
<th>Failure Strain [%]</th>
<th>Modulus [GPa]</th>
<th>Poisson's Ratio</th>
<th>PEL Strain [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>Mean</td>
<td>Standard Deviation</td>
<td>Mean</td>
<td>Standard Deviation</td>
<td>Mean</td>
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<td></td>
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Figure 4.10 displays the principal strain fields of transverse tension specimens at room and hot conditions, where the arrows indicate the principal strain directions. The strain field on the transverse specimens is nonuniform with a distinct local strain pattern evident along the edges of the specimen for room as well as environmentally conditioned tests. The periodic strain pattern consists of a set of two high, closely spaced strain areas followed by a large semi-circular area of low strain. Other researchers have noted similar patterns using the out-of-plane deformation field (Roberts et al., 2009; C. Zhang & Binienda, 2014) and the uniaxial strain field (Kohlman et al., 2012; Littell et al., 2009; Roberts et al., 2009) for room condition. Zhang and Binienda (2014) concluded that the pattern is caused by tension-torsion coupling due to the termination of bias braid tows at the edges of the specimen. The principal strain directions in the zoomed-in area of the transverse tensile
strain field in Figure 4.10 show this edge effect. It is important to state that similar strain patterns are evident for each environmental condition. However, the strain level at the initial macroscopic damage as well as the intensity and size of the edge effects can differ between room and environmental conditions as discussed later. The surface and through-thickness images of the failed specimens depicted in Figure 4.11 show shear failure along the bias braid tows of transverse tensile specimens. Additionally, from observing the tests and analyzing the failure of the specimens, it is clear that the resistance to shear along the bias tow reduces with environmental conditioning, yielding less destructive failure events.
Figure 4.10. Contours Showing the Principal Strain Field of Transverse Tensile Specimens Just Before Failure for (a) the Room Condition and (b) the Hot Condition
Figure 4.11. Photos Showing the Failure of Transverse Tensile Specimens Under Different Environmental Conditions

The principal strain fields of axial tension specimens at room and hot/wet conditions are displayed in Figure 4.12. The strain field on the axial specimen is nonuniform with local high strain areas occurring in relatively equal frequency at the edges and center of the specimen. The principal strain directions show that the global strain was mostly parallel to the direction of loading, even in the local high strain areas, and the edges of the axial specimens had almost no effect on the principal strain directions. Surface images, presented in Figure 4.13, show fiber breakage in the axial tows of axial tension specimens
which causes several bias tows to pull out from the specimen. Comparison of the tests at room and environmental conditions shows that failure occurs at lower stresses and strains for the axial tensile tests under environmental conditions, but each condition has common failure mechanisms.

Figure 4.12. Contours Showing the Principal Strain Field of Axial Tensile Specimens Just Before Failure for (a) the Room Condition and (b) the Hot/Wet Condition
In order to quantify the effect of environmental conditions on the strain patterns and edge effects, a through-width strain distribution analysis was conducted. The principal strain distribution was investigated at multiple cross sections by plotting the strain as a function of specimen width. The through-width strain data for each environmental condition was extracted at a stage corresponding to the PEL strain in order to study macroscopic damage initiation. The strain distribution at the PEL point is used to compare and investigate the possible causes of nonlinearity at different environmental conditions in addition to the strain pattern and edge effects. The principal strain results are presented as a function of width (Figure 4.14) for transverse tension specimens at each environmental condition.
condition where the black curves represent the strain data extracted from sections of the strain field. The data was discretized with blue circular points representing the principal strain at the edges of the specimen where large strain gradients are prominent and red triangular points representing the strain at the center of the specimen where the values are approximately constant. The data provided from this analysis was used to compute $\alpha$ (indicating strain concentration) and $\beta$ (indicating size of the edge effect) parameters which are defined by Equations (4.4) and (4.5), respectively. It must be noted that parameter $\beta$ describes a ratio that directly represents the physical size of the edge effects, whereas parameter $\alpha$ complements $\beta$ by defining the intensity of the edge strain. Therefore, changes in the size of edge effects due to environmental conditions are better represented by the values of $\beta$. An additional parameter, $\eta$, is defined to effectively account for the size of the edge effects as well as for the intensity. The parameter $\eta$, described in Equation (4.6), integrates the edge and center strain in the strain-width plots (Figure 4.14).

$$\alpha = \frac{\bar{\varepsilon}_{\text{edge}}}{\bar{\varepsilon}_{\text{center}}}$$  \hspace{2cm} (4.4)

$$\beta = \frac{W_{\text{edge}}}{W_{\text{center}}}$$  \hspace{2cm} (4.5)

$$\eta = \frac{\int_{0}^{d_{\text{left}}} \varepsilon_{\text{edge}}(x) \, dx + \int_{d_{\text{right}}}^{d_{\text{specimen}}} \varepsilon_{\text{edge}}(x) \, dx}{\int_{d_{\text{left}}}^{d_{\text{right}}} \varepsilon_{\text{center}}(x) \, dx}$$  \hspace{2cm} (4.6)

In Equations (4.4) and (4.5), $\bar{\varepsilon}_{\text{edge}}$ and $\bar{\varepsilon}_{\text{center}}$ represent the average values of principal strain at the edges and the center of the specimen, respectively, and $W_{\text{edge}}$ and $W_{\text{center}}$ are
the average calculated widths of the edge strain and center strain, respectively. The $d_{left}$ and $d_{right}$ variables defined in Equation (4.6), and illustrated in Figure 4.14(a), are determined by the calculated strain gradient and represent transition points in the strain-width plots; the $d_{specimen}$ variable represents the width of the specimen. The strain distribution parameters, $\alpha$, $\beta$, and $\eta$, for the axial and transverse tensile specimens are provided in Table 4.4. The parameter ratios, as well as the strain-width plots in Figure 4.15, show that the edge effects for the axial tension specimens are small and unaffected by the environmental conditions. On the contrary, the strain-width plots in Figure 4.14 and the parameter ratios convey that the edge effects are critical and large for the transverse tension specimens at environmental conditions. The $\eta$ ratios have similar trends to the $\beta$ ratios but are slightly larger in value for the transverse tensile response. The possible causes for the larger size of edge effects in the transverse tensile specimens due to environmental conditions are increases in tow splitting damage.
Figure 4.14. Strain-Width Plots for Transverse Tensile Specimens
Table 4.4. Average Tension Strain Distribution Results

<table>
<thead>
<tr>
<th>Specimen Type</th>
<th>Parameter</th>
<th>Room</th>
<th>Hot</th>
<th>Hot/Wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial Tension</td>
<td>$\alpha$</td>
<td>1.00</td>
<td>0.95</td>
<td>1.06</td>
</tr>
<tr>
<td></td>
<td>$\beta$</td>
<td>0.05</td>
<td>0.07</td>
<td>0.09</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>0.02</td>
<td>0.03</td>
<td>0.05</td>
</tr>
<tr>
<td>Transverse Tension</td>
<td>$\alpha$</td>
<td>1.30</td>
<td>1.22</td>
<td>1.28</td>
</tr>
<tr>
<td></td>
<td>$\beta$</td>
<td>0.24</td>
<td>0.41</td>
<td>0.77</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>0.27</td>
<td>0.42</td>
<td>0.80</td>
</tr>
</tbody>
</table>

The bowtie specimens were originally designed to mitigate the edge effects present in the transverse tension specimens (Bowman et al., 2003). The design of the notch for the bowtie specimen follows the angle of the braid to decrease the probability of a bias braid tow terminating at the edge. The principal strain field in Figure 4.16(a) demonstrates that the edge effects along the specimen are minimal but concentrations still occur in the gage.
area near the notch tip due to the specimen geometry. The through-thickness and surface images illustrate failure associated with fiber breakage in the bias braid tows. The elastic and failure properties presented in Table 4.5 and the stress-strain plots of the bowtie specimens in Figure 4.17 show that the bowtie moduli are larger than the axial and transverse moduli of the straight sided specimens due to the complex tow architecture. The braid angle and lack of tow continuity between the top and bottom grip surfaces in the transverse tension specimen reduce the elastic modulus. In contrast to the transverse tension straight sided specimen, bowtie specimens have tow continuity which allows the specimen to distribute the applied stress more effectively through the bias braid tows and provides larger strength values. The approximate schematic in Figure 4.18 illustrates the tow continuity between grip surfaces for the bowtie specimens as well as the bias braid termination that occurs in the transverse tensile straight-sided specimens. The architecture of the material is presented in Figure 4.19; this cross section shows that the transverse direction contains more bias braid tows compared to the number of axial tows in the axial direction. The tow continuity and larger number of bias tows produce the larger moduli measurements for the bowtie tests. The results in this chapter and previous studies (Bowman et al., 2003; Kohlman et al., 2012) show that another potential cause of the irregular moduli values is the multiaxial stress state at the notch of the specimen.
Figure 4.16. (a) Principal Strain Field and Directions and (b) Surface and Through-Thickness Failure Modes of a Hot Conditioned Bowtie Specimen

Table 4.5. Bowtie Mechanical Properties

<table>
<thead>
<tr>
<th>Condition</th>
<th>Material Parameter</th>
<th>Mean</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room Condition</td>
<td>Failure Stress [MPa]</td>
<td>825.75</td>
<td>53.32</td>
</tr>
<tr>
<td></td>
<td>Modulus [GPa]</td>
<td>64.32</td>
<td>5.37</td>
</tr>
<tr>
<td>Hot</td>
<td>Failure Stress [MPa]</td>
<td>790.54</td>
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<td>Modulus [GPa]</td>
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<td>Hot/Wet</td>
<td>Failure Stress [MPa]</td>
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<td></td>
<td>Modulus [GPa]</td>
<td>58.26</td>
<td>7.75</td>
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</table>
Figure 4.17. Stress-Strain Plots for Each Transverse Bowtie Tensile Specimen

Figure 4.18. Bias Braid Tows in Bowtie and Transverse Tension Specimens
4.4.2. Compressive Response

Transverse and axial stress-strain plots for each tested compression specimen are presented in Figure 4.20 and Figure 4.21, respectively. Unlike the axial tensile response, the axial compression stress-strain response shows nonlinear behavior. The principal strain field and images of failure modes presented in Figure 4.22 show that the nonlinearity of the axial compression specimen was not caused by edge effects. The nonlinearity of the axial compression specimens is attributed to the fiber microbuckling and shear failure modes which were not present in the axial tension specimens. The principal strain contours show the existence of concentrations in the transverse compression specimen; although, these concentrations were not specifically located along the edge as in the transverse tension results. Furthermore, the through-width strain distribution results in Table 4.6 and strain-width plots in Figure 4.23 demonstrate that, similar to the axial tensile results, the size of the edge effects in the compression specimens are small with minimal changes due to the environmental conditions. The PEL strains for the axial and transverse compression response, presented in Table 4.7, show that the environmental conditions cause damage at lower strains. The axial and transverse compressive strength, failure strain, modulus, and
Poisson’s ratio are also summarized in Table 4.7. With the exception of the modulus, significant degradation of the mechanical properties was prevalent due to the environmental conditions.

Figure 4.20. Stress-Strain Plots for Each Transverse Compression Specimen

Figure 4.21. Stress-Strain Plots for Each Axial Compression Specimen
Figure 4.22. Principal Strain Contours and Failure Images of Hot/Wet Conditioned Axial and Transverse Compression Tests

<table>
<thead>
<tr>
<th>Specimen Type</th>
<th>Parameter</th>
<th>Room</th>
<th>Hot</th>
<th>Hot/Wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial Compression</td>
<td>$\alpha$</td>
<td>1.4</td>
<td>1.25</td>
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<tr>
<td></td>
<td>$\beta$</td>
<td>0.11</td>
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</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>0.08</td>
<td>0.11</td>
<td>0.13</td>
</tr>
<tr>
<td>Transverse Compression</td>
<td>$\alpha$</td>
<td>2.8</td>
<td>2.4</td>
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<tr>
<td></td>
<td>$\beta$</td>
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<td>0.14</td>
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<tr>
<td></td>
<td>$\eta$</td>
<td>0.18</td>
<td>0.21</td>
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Figure 4.23. Strain-Width Plots for Axial and Transverse Compression Specimens
Table 4.7. Compression Mechanical Properties

<table>
<thead>
<tr>
<th>Condition</th>
<th>Material Parameter</th>
<th>Axial Compression</th>
<th>Transverse Compression</th>
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</thead>
<tbody>
<tr>
<td>Room Condition</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>Failure Stress [MPa]</td>
<td>441.50</td>
<td>370.67</td>
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<td></td>
<td>Standard Deviation</td>
<td>39.52</td>
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<td></td>
<td>Failure Strain [%]</td>
<td>1.37</td>
<td>0.98</td>
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<td></td>
<td>Standard Deviation</td>
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<td>0.11</td>
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<tr>
<td></td>
<td>Modulus [GPa]</td>
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<td></td>
<td>Standard Deviation</td>
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<td></td>
<td>Poisson's Ratio</td>
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<td>0.33</td>
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<td></td>
<td>Standard Deviation</td>
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<td>0.01</td>
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<tr>
<td></td>
<td>PEL Strain [%]</td>
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<td>Standard Deviation</td>
<td>0.10</td>
<td>0.08</td>
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<tr>
<td>Hot</td>
<td>Failure Stress [MPa]</td>
<td>286.14</td>
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<td></td>
<td>Standard Deviation</td>
<td>62.94</td>
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<tr>
<td></td>
<td>Failure Strain [%]</td>
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<td>Standard Deviation</td>
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<td></td>
<td>Modulus [GPa]</td>
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<td>39.00</td>
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<td>Standard Deviation</td>
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<td>Poisson's Ratio</td>
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<td>Standard Deviation</td>
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<td></td>
<td>PEL Strain [%]</td>
<td>0.59</td>
<td>0.70</td>
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<tr>
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<td>Standard Deviation</td>
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<td>0.06</td>
</tr>
<tr>
<td>Hot/Wet</td>
<td>Failure Stress [MPa]</td>
<td>267.04</td>
<td>258.39</td>
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<tr>
<td></td>
<td>Standard Deviation</td>
<td>29.13</td>
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<td></td>
<td>Failure Strain [%]</td>
<td>0.76</td>
<td>0.66</td>
</tr>
<tr>
<td></td>
<td>Standard Deviation</td>
<td>0.10</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>Modulus [GPa]</td>
<td>37.75</td>
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</tr>
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<td></td>
<td>Standard Deviation</td>
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<tr>
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<td>Poisson's Ratio</td>
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<td>0.38</td>
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<td></td>
<td>Standard Deviation</td>
<td>0.03</td>
<td>0.12</td>
</tr>
<tr>
<td></td>
<td>PEL Strain [%]</td>
<td>0.63</td>
<td>0.62</td>
</tr>
<tr>
<td></td>
<td>Standard Deviation</td>
<td>0.07</td>
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</tr>
</tbody>
</table>

4.4.3. V-Notched Rail Shear Response

The nonlinear stress-strain plots for the shear specimens are shown in Figure 4.24 and the corresponding elastic and failure properties are presented in Table 4.8. The presented shear properties for the room condition correlate well with the v-notched rail shear results obtained by Roberts et al. (2009). The calculated PEL strains for the shear response were largely unaffected by the environmental conditioning of the specimens. The results show that the environmental conditions significantly affect the failure strength with only minor effects on the failure strain and shear modulus. Due to the limited DIC viewing area of the shear specimen, the through-width strain distribution analysis was not performed for this response.
Table 4.8. In-Plane Shear Mechanical Properties

<table>
<thead>
<tr>
<th>Condition</th>
<th>Material Parameter</th>
<th>Mean</th>
<th>Standard Deviation</th>
</tr>
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<tbody>
<tr>
<td>Room Condition</td>
<td>Failure Stress [MPa]</td>
<td>255.78</td>
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<tr>
<td></td>
<td>Failure Strain [%]</td>
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<tr>
<td></td>
<td>Modulus [GPa]</td>
<td>17.56</td>
<td>1.19</td>
</tr>
<tr>
<td></td>
<td>PEL Strain [%]</td>
<td>1.18</td>
<td>0.21</td>
</tr>
<tr>
<td>Hot</td>
<td>Failure Stress [MPa]</td>
<td>186.84</td>
<td>14.18</td>
</tr>
<tr>
<td></td>
<td>Failure Strain [%]</td>
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<td>0.22</td>
</tr>
<tr>
<td></td>
<td>Modulus [GPa]</td>
<td>16.22</td>
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<tr>
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<td>PEL Strain [%]</td>
<td>0.80</td>
<td>0.19</td>
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<td>Hot/Wet</td>
<td>Failure Stress [MPa]</td>
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<tr>
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<td>Failure Strain [%]</td>
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<td>0.19</td>
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<td>Modulus [GPa]</td>
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<td>1.74</td>
</tr>
<tr>
<td></td>
<td>PEL Strain [%]</td>
<td>1.01</td>
<td>0.18</td>
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</tbody>
</table>
4.4.4. Damage and Failure Analysis

In addition to the complete failure of a component or specimen, intermediate damage induced by mechanical loading and environmental conditions changes the composite structure and causes degradation of the material properties. Several load/unload tests were performed to capture this modulus degradation in individual axial and transverse tensile specimens at the room condition. The testing was conducted at the same displacement rate as the previously mentioned tests but consisted of three distinct phases: i) loading, ii) unloading, and iii) reloading. In the first phase, the specimens were loaded to a stress corresponding to approximately 85% of the average failure strength for the axial and transverse tensile properties (Table 4.3). The applied stress was removed during the unloading phase by reversing the direction of the displacement rate. These phases are depicted in Figure 4.25 using axial and transverse tensile stress-strain plots; the calculated moduli are also shown. The ratio of the reloading modulus to the loading modulus for each case indicates the occurrence of damage and structural changes in the material. The moduli ratio for the axial tension specimens is smaller than the transverse tension ratio, demonstrating that more structural change and damage occurs due to the transverse tensile specimen geometry. This degradation shows the importance of utilizing nondestructive evaluation and microscopy techniques for the characterization of damage.
Failure analysis was performed using a pulsed flash thermography technique which uses two bulbs to apply heat to the surface of a specimen and an infrared camera to capture temperatures contours of the specimen. In order to accurately analyze the failed and damaged specimens, two unconditioned, untested specimens (defined as healthy specimens) were placed under the infrared camera to obtain reference data points. The EchoTherm software compiles images of the temperature contours of the specimens at specific time intervals during and after the flash from the bulbs. As shown in Figure 4.26(a) and Figure 4.27(a), the temperature data is computed from specific areas called cursors using the EchoTherm software and multiple cursors were used in random locations at the center of the specimen to average and extract data from the healthy and failed/damaged specimens. Information regarding flash thermography and the EchoTherm software can be found in the ASTM E2582 (2007) standard and the EchoTherm manual (Thermal Wave
Additionally, multiple pulsed flashes and data collection were conducted in order to get an appropriate number of data points for each damaged/failed specimen. For the failed specimens, the cursor windows were placed over areas immediately adjacent to the failure region in order to determine the impact of loading on the overall structure of the specimen. The initial temperature value from each cursor window was subtracted from the subsequent values and logarithmic temperature-time plots were made to visualize the difference in thermography results between healthy and failed/damaged specimens (Figure 4.26b and Figure 4.27b). Following the ASTM E2582 standard, a line with a slope of -0.5 is overlaid starting at the descent of these curves and any deviations from this slope represent defects/damage within the material. For the current analysis, the area under the temperature-time curves was used. The ratio of healthy area to damaged area at the center of each specimen is defined as the central damage parameter. The damage metric was also applied to determine the effects that environmental conditioning and loading have at the edges of the specimen (referred to as the edge/center damage parameter). This edge/center damage value is the ratio of the edge area to the central area of the temperature-time plot where the edge area was extracted using cursor windows placed near the edge of the specimens.
Figure 4.26. (a) Multiple Cursor Windows Overlaid on a Flash Thermography Contour and (b) a Logarithmic Plot of Temperature-Time Data for Healthy and Failed Axial Compression Specimens

Figure 4.27. (a) Multiple Cursor Windows Overlaid on a Flash Thermography Contour and (b) a Logarithmic Plot of Temperature-Time Data for Healthy and Damaged Axial Compression Specimens
Several specimens were loaded to intermediate stress levels to induce damage without failure. These results were then used to better quantify damage progression. The edge/damage ratio for the healthy state was approximately 1.24 and this initial concentration was caused by damage induced during fabrication of the specimens and also due to boundary effects during the flash thermography procedure. The healthy state of a specimen has a value of 100% and any deviations from this value represent center damage in the specimen. The deviations in the edge/center ratios (shown in Figure 4.28) for the damaged axial tension specimens demonstrate negligible effects due to the edges. These edge/center ratios verify the through-width strain distribution results in Table 4.4 and indicate that premature damage due to tow splitting was not apparent. For the failed specimens at room and environmental conditions, the edge/center ratios increased above 1.4 likely due to stress waves caused by the sudden failure of the specimen. The flash thermography analysis for the transverse tensile specimens (Figure 4.29) shows markedly different trends than that of the axial tension. The transverse tensile results show larger edge/center ratios between the damaged and healthy states. Specifically, the results show larger edge/center ratios for specimens loaded to PEL and after PEL which indicate the occurrence of progressive damage at the edge of the specimen potentially due to increased splitting of the subsurface axial tows. The increased edge/center ratios correlate with the through-width strain distribution results in Table 4.4, evidence that strain concentrations occur at the edges of specimens loaded to the PEL point. A comparison of the environmental conditions with the room condition demonstrates that, for similar stress levels, the environmental conditions had larger edge/center ratios. The central damage percentages show that specimens at environmental conditions were more susceptible to
damage compared to the specimens at room condition. Flash thermography analysis for axial and transverse compression specimens are displayed in Figure 4.30 and Figure 4.31, respectively, and the results illustrate trends comparable to the tension. However, the central damage parameter for several of the failed compression specimens demonstrates that more damage was induced compared to the values of the transverse tension.

Figure 4.28. Thermography Analysis of the Axial Tensile Specimens
Figure 4.29. Thermography Analysis of the Transverse Tensile Specimens

Figure 4.30. Thermography Analysis of the Axial Compression Specimens
Scanning electron microscopy was performed on damaged and failed transverse tensile specimens to study damage initiation and propagation in the material. Figure 4.32(a) shows a low magnification image of a damaged specimen at the room condition with tow splitting in several locations. A higher magnification micrograph of one of these tow splitting sites (Figure 4.32b) better depicts the phenomena and shows the initiation of tow debonding. Figure 4.33(a) and (b) show similar tow splitting for a damaged specimen at the hot condition but the tow debonding for this condition is more prominent and the damage is achieved with less applied stress. For a failed specimen at the hot condition (Figure 4.33c) tow splitting, tow debonding, and fiber debonding are mechanisms that
contributed to failure. The fiber structure, shown by a high magnification image of the interior of a tow splitting site (Figure 4.33d), indicates that this particular tow split initiated at the edges of the specimen due to a concentration that occurred during testing or due to a pre-existing defect. The damage and failure mechanisms for a specimen at the hot/wet condition (Figure 4.34) are similar to the specimen at the hot condition. The micrographs for each condition show that tow splitting and debonding are principal failure mechanisms for this material.

![Image](image1.jpg)

(a) Loaded to 425 MPa (35x)  
(b) Loaded to 425 MPa (100x)

![Image](image2.jpg)

(c) Failed (30x)  
(d) Failed (500x)

Figure 4.32. Scanning Electron Microscopy Images of Transverse Tensile Specimens Tested Under Room Condition
Figure 4.33. Scanning Electron Microscopy Images of Transverse Tensile Specimens Tested Under Hot Condition

(a) Loaded to 310 MPa (50x)
(b) Loaded to 310 MPa (350x)
(c) Failed (30x)
(d) Failed (200x)

Figure 4.34. Scanning Electron Microscopy Images of Transverse Tensile Specimens Tested Under Hot/Wet Condition

(a) Loaded to 260 MPa (30x)
(b) Failed (30x)
4.5. Chapter Summary

This chapter examined the effects of hot (100°C) and hot/wet conditions (60°C/90% relative humidity) on the mechanical properties and failure of triaxial braided composites under tension, compression, and shear. A humidity and temperature controlled chamber was used to condition the hot/wet conditioned specimens. An in-situ thermal chamber heated the hot and hot/wet conditioned specimens to 100°C during the mechanical testing. The volume fraction tests were conducted on multiple triaxial braided composite panels to obtain a statistical range for the material. Strain measurements were made, during mechanical loading, using a DIC system. Damage and failure analyses were performed using a non-destructive, flash thermography system and a scanning electron microscope. The following conclusions and results are made from analysis of the experiments:

1. A decrease in failure stress by approximately 20% was observed for tension, compression, and shear when comparing the environmental conditions to the room condition baseline.

2. Additionally, a decrease in modulus was apparent for the transverse tension, bowtie, and shear specimens under environmental conditions.

3. The through-width strain distribution results demonstrated that strain concentrations exist on the edges, and the size of these edge effects increases with environmental conditions.

4. The through-width strain results were verified with the flash thermography analysis, which inspected the damage in the center and at the edges of each specimen.
5. The scanning electron microscopy showed similar damage propagation mechanisms for both hot and hot/wet conditions. Damage was shown to initiate in the form of tow splitting, and total failure was a combination of failure modes, including tow splitting, tow debonding, and fiber debonding.

6. The overall conclusions from the experiments show that an increase in temperature is a driving factor for the degradation of the material parameters.
5. MULTISCALE MODELING OF TRIAXIAL BRAIDED COMPOSITES
INCLUDING TEMPERATURE AND MOISTURE EFFECTS

5.1. Introduction

Understanding the effect of triaxial braided composites under environmental conditions is important for the design of aerospace components. However, experimental testing is time consuming and expensive. Therefore, the ability to model and reliably analyze triaxial braided composites is a key step to understanding the applicability of the designed material. The extreme environment subjected on aerospace components requires the consideration of these conditions in modeling techniques. The modeling of the triaxial braided material under environmental conditions is also challenging due to the complex 3D architecture. A multiscale modeling framework for triaxial braided composite materials is developed in this chapter to capture the micro- and mesoscale structure of the material and scale the behavior to the macroscale. For the microscale, the various defined microstructures are simulated using the high fidelity micromechanics method detailed in Chapter 3. Temperature and moisture terms are added to the constitutive laws for the individual composite constituents. The mesoscale model is constructed by defining different fiber volume fractions and 3D tow orientations to mesoscale subcells. The final macroscale model is created in LS-DYNA (Hallquist, 2007) by repeating several mesoscale unit cells to replicate axial and transverse tension specimen geometry. The experimental results from the room and hot/wet (60°C/ 90% Relative Humidity) conditions in Chapter 4 are used to validate the axial and transverse tension simulations.
5.2. Multiscale Triaxial Model

5.2.1. High Fidelity Micromechanics

The HFGMC theory overviewed and described in Chapter 3.1.1 is utilized in the multiscale model to generate the effective material properties for the mesoscale subcells. The different environmental conditions are addressed by incorporating coefficient of thermal, $\alpha^{(\text{subind})}$, and moisture, $\beta^{(\text{subind})}$, expansion terms within the constitutive laws in Equation (3.28) and (3.29). These constitutive laws with environmental effects are defined in Equation (5.1) for the fiber subcells and Equation (5.2) for the polymer subcells, where $\Delta T$ and $\Delta M$ represent the changes in temperature and moisture absorption of the material, respectively. The room and hot/wet (60°C/ 90% Relative Humidity) conditions from Chapter 4 are used in the microscale simulations.

\[
\sigma^{(\text{subind})}_{ij} = C_{ijkl}^{(\text{subind})} \left( \epsilon^{(\text{subind})}_{ij} - \alpha^{(\text{subind})} \Delta T \right) \quad (5.1)
\]

\[
\sigma^{(\text{subind})}_{ij} = C_{ijkl}^{(\text{subind})} \left( \epsilon^{(\text{subind})}_{ij} - \epsilon^{(\text{subind})}_{ij} - \alpha^{(\text{subind})} \Delta T - \beta^{(\text{subind})} \Delta M \right) \quad (5.2)
\]

The inelastic strains of the isotropic polymer subcells are calculated from the viscoplastic theory detailed in Chapter 2. The fiber subcells are represented as transversely isotropic, linear elastic material. The triaxial braid composite consists of PR-520 polymer resin and T700S carbon fibers, and the mechanical properties for the constituents are presented in Table 5.1 and Table 5.2. The moisture absorption is assumed to be solely concentrated in the polymer matrix; thus, a coefficient of moisture expansion is not assigned to the fiber. The elastic and viscoplastic properties for the PR-520 polymer resin are obtained from Goldberg et al. (2005). Although only the elastic properties are extracted and scaled to the mesoscale, the viscoplastic law is useful for determining the elastic range.
for each loading direction and unit cell. It is important to note that the $\alpha$ symbol is used to denote considerably different types of polymer properties where $\alpha_0$ and $\alpha_1$ represent the initial and final values, respectively, of the internal hydrostatic state variable in the viscoplastic law, $\alpha_m$ represents the coefficient of thermal expansion for the polymer matrix, and $\alpha_{1f}$ and $\alpha_{2f}$ denote the coefficient of thermal expansion for the fiber in the axial and transverse directions, respectively. Three microscale unit cells (Figure 5.1) are created to represent the different $V_f$ specifications of the mesoscale RUC and further details of these specifications are presented in the following subsection.

<table>
<thead>
<tr>
<th>Property:</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{11}$ (GPa)</td>
<td>230</td>
</tr>
<tr>
<td>$E_{22}$ (GPa)</td>
<td>15</td>
</tr>
<tr>
<td>$G_{12}$ (GPa)</td>
<td>24</td>
</tr>
<tr>
<td>$G_{23}$ (GPa)</td>
<td>5.03</td>
</tr>
<tr>
<td>$\nu_{12}$</td>
<td>0.20</td>
</tr>
<tr>
<td>$\nu_{23}$</td>
<td>0.20</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>1800</td>
</tr>
<tr>
<td>$\alpha_{1f}$ (1/°C)</td>
<td>-0.38E-6</td>
</tr>
<tr>
<td>$\alpha_{2f}$ (1/°C)</td>
<td>11.0E-6</td>
</tr>
</tbody>
</table>
Table 5.2. Material Properties for PR-520 Epoxy

<table>
<thead>
<tr>
<th>Property</th>
<th>Value 1</th>
<th>Value 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>3.54 ($\dot{\varepsilon} = 7 \times 10^{-5}$ s$^{-1}$)</td>
<td>3.54 ($\dot{\varepsilon} = 1.76$ s$^{-1}$)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.38</td>
<td></td>
</tr>
<tr>
<td>$D_0$</td>
<td>1.00E6</td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>0.93</td>
<td></td>
</tr>
<tr>
<td>$Z_0$ (MPa)</td>
<td>396.09</td>
<td></td>
</tr>
<tr>
<td>$Z_1$ (MPa)</td>
<td>753.82</td>
<td></td>
</tr>
<tr>
<td>$q$</td>
<td>279.26</td>
<td></td>
</tr>
<tr>
<td>$\alpha_0$</td>
<td>0.568</td>
<td></td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>0.126</td>
<td></td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>1256</td>
<td></td>
</tr>
<tr>
<td>$\alpha_m$ ($1/°C$)</td>
<td>52.9E-6</td>
<td></td>
</tr>
<tr>
<td>$\beta_m$ ($1/%H_2O$)</td>
<td>3.24E-3</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.1. Microscale Unit Cell Geometries with Different $V_f$ Specifications

5.2.2. Mesoscale Unit Cell

The mesoscale structure models the triaxial braided composite through an RUC that is discretized both in-plane and through-thickness of the material. The subcell discretization scheme from the absorbed matrix model (AMM) developed by Cater et al. (2013) is utilized in the current mesoscale model. The AMM performs in-plane
discretization of a single layer of triaxial material which creates the four sections illustrated in Figure 5.2. Further discretization is performed through-thickness to create the final geometry of the mesoscale subcells, which are considered to be sequences of unidirectional laminae with different $V_f$ specifications and tow orientations. The current mesoscale model assigns five subcell definitions from this discretized geometry as shown in Figure 5.3. The additional two subcells (Subcells 3 and 4) specify an undulation angle. Figure 5.3 also introduces a subcell shift rule for model development where the RUC is stacked to form a two-RUC volume with the second RUC volume shifted in-plane by one mesoscale subcell. The purpose of this shift is to accurately represent the physical mesoscale tow structure of the material by ensuring that an axial tow is always present in a through-thickness slice of the model.

Figure 5.2. In-Plane Discretization of the Mesoscale RUC

Figure 5.3. Schematics Showing Mesoscale RUC
The specifications for the five mesoscale subcells are presented in Table 5.3. The $V_f$ values from the AMM are applied and the tow undulation angle was measured using microscopy. Since the triaxial material has a large tow structure, the microscopy analysis was conducted using a Zeiss laser scanning microscope (LSM 700) and multiple micrographs were stitched together to form a mosaic as shown in Figure 5.4. The mesoscale subcells in the current model are integrated as solid elements in the macroscale LS-DYNA simulation. In contrast, the AMM performs through-thickness homogenization using classical laminate theory yielding four effective mesoscale subcells which are applied to shell elements in a finite element analysis. The disadvantage of the shell element formulation is that tow undulation cannot be properly accounted for in the effective properties of the mesoscale subcells.

<table>
<thead>
<tr>
<th>Table 5.3. Subcell Angle Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subcell 1</td>
</tr>
<tr>
<td>$V_f$ (%)</td>
</tr>
<tr>
<td>Braid Angle (deg.)</td>
</tr>
<tr>
<td>Undulation (deg.)</td>
</tr>
</tbody>
</table>

Figure 5.4. Mosaic of the Triaxial Architecture
5.2.3. Macroscale Model

The shifted RUC was projected in each direction to fit the width and thickness dimensions of the axial and transverse tension specimens used in the experiments. For the axial tension specimen, the thickness is 3.24 mm, the width is 31.09 mm, and the length is 280.5 mm as shown in Figure 5.5(a). The specimen model presented in Figure 5.5(a) represents a coarse mesh of the geometry (5,775 elements) where each solid element is a mesoscale subcell. Different mesh refinements of the axial tension specimen are also studied and the refined meshed geometry in Figure 5.5(b) is achieved by splitting the length and width of the elements in the coarse mesh. Since the through-thickness dimensions of the elements in the original mesh are comparably smaller, the refinement is not performed through-thickness. This refinement method is also performed on the 23,100 element mesh to obtain the finer mesh depicted in Figure 5.5(c) which is 92,400 elements. Using the same element refinement scheme, three meshes for the transverse tension specimen are also created (Figure 5.6). The inconsistency in the dimensions and the number of elements between the axial and transverse tension models is related to the irregular aspect ratio of the mesoscale RUC.

![Diagram of specimen model with dimensions and element counts](image-url)
Figure 5.5. Axial Tensile Specimen Models with Varying Mesh Refinements

Figure 5.6. Transverse Tensile Specimen Models with Varying Mesh Refinements
The boundary conditions and loadings in the specimen models simulate the conditions that the physical specimens experienced during the mechanical testing. The gripping length of the physical specimens is replicated by selecting all the nodes within a length of 40.8 mm at each end for the axial specimen model (Figure 5.7a) and 40.1 mm at each end for the transverse specimen model (Figure 5.7b). The accurate simulation of the gripping length also ensures that the gage length in the models is the same as that of the experiments. The nodes selected at one end are fixed with all the 3D displacement and rotations constrained. The nodes selected at the other end of the specimen are given a translational displacement by using the *PRESCRIBED_MOTION_SET keyword in LS-DYNA. The boundary conditions and translational displacements are the same for both the axial and transverse tension specimens with the exception that the x-translational displacement degree of freedom is selected for the axial model and the y-translational displacement is designated for the transverse model. The simulated translational displacements correlate with the 0.025 inch/min displacement rate used for the experiments.

![Diagram of Axial Tension Conditions](image)

(a) Axial Tension Conditions
Five separate orthotropic elastic material keywords are created to represent the different mesoscale subcells where the material axes are defined using the global coordinate system. The material properties, for each orthotropic elastic keyword, are obtained from the results of the micromechanics simulations which are presented later in this chapter. These material properties are different between the room and hot/wet conditions since temperature and moisture terms effect the microscale generated properties. The coordinate system for each material is defined by computing a set of vectors using the tow angle specifications from Table 5.3. Figure 5.8 illustrates these material vectors for each subcell, in the global coordinate system, where $A$ is the vector aligned with the tow in the subcell and $D$ is a vector perpendicular to the tow. The $\theta$ and $\phi$ symbols denote the braid and undulation angles, respectively. The values for the material unit vector components are presented in Table 5.4 and the subscripts indicate the component direction with respect to the global coordinate system. For the transverse model with the highest refined mesh, two different versions are made for comparison, one with undulation and one without undulation. Subsequently, for the version without undulation, the $A$ and $D$ vectors
for Subcell 3 and Subcell 4 become the same vectors designated for Subcell 2 and Subcell 1, respectively.

![Figure 5.8: Material Axes Defined for Each Mesoscale Subcell in the Global Coordinate System](image)

Table 5.4. Material Unit Vector Components

<table>
<thead>
<tr>
<th></th>
<th>Subcell 1</th>
<th>Subcell 2</th>
<th>Subcell 3</th>
<th>Subcell 4</th>
<th>Subcell 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_x$</td>
<td>0.500</td>
<td>0.500</td>
<td>0.447</td>
<td>0.447</td>
<td>1.000</td>
</tr>
<tr>
<td>$A_y$</td>
<td>0.866</td>
<td>-0.866</td>
<td>-0.774</td>
<td>0.774</td>
<td>0</td>
</tr>
<tr>
<td>$A_z$</td>
<td>0</td>
<td>0</td>
<td>-0.448</td>
<td>0.448</td>
<td>0</td>
</tr>
<tr>
<td>$D_x$</td>
<td>-0.866</td>
<td>0.866</td>
<td>0.888</td>
<td>-0.457</td>
<td>0</td>
</tr>
<tr>
<td>$D_y$</td>
<td>0.500</td>
<td>0.500</td>
<td>0.325</td>
<td>0.628</td>
<td>1.000</td>
</tr>
<tr>
<td>$D_z$</td>
<td>0</td>
<td>0</td>
<td>0.325</td>
<td>-0.629</td>
<td>0</td>
</tr>
</tbody>
</table>

5.3. Simulations Results and Discussion

5.3.1. Microscale Results

The mesoscale subcells are assumed to be transversely isotropic, unidirectional layers with various material properties and orientations. Thereby, micromechanics simulations are performed for each type of unidirectional layer to obtain the five necessary material properties: $E_{11}$, $E_{22}$, $G_{12}$, $\nu_{12}$, and $\nu_{23}$. These properties are obtained for each microscale
unit cell geometry by conducting simulations using axial, transverse, and in-plane shear loadings. Figure 5.9 shows the stress-strain responses for the axial (11) tension loading of the microscale unit cells with different fiber volume fractions and conditions. The room condition results show large stiffness for the unit cells with $V_f$ values of 80% and 73.3% and a significantly smaller stiffness for the unit cell simulation with 37.5% fiber volume fraction. A comparison of the room and hot/wet condition shows that the hot/wet condition causes a decrease in stiffness for each unit cell. The plots of the unit cell simulations with the transverse (22) tension loading in Figure 5.10 display similar trends as the axial tension results, except the transverse results have increased nonlinear behavior. The elastic properties for each unit cell $V_f$ specification, environmental condition, and mechanical loading are extracted from a strain range of 0.1% to 0.25% and a summary of these properties is presented in Table 5.5.

![Figure 5.9. Stress-Strain Response for Axial (11) Loading of Unit Cells with Different $V_f$ Specifications](image-url)
Figure 5.10. Stress-Strain Response for Transverse (22) Loading of Unit Cells with Different $V_f$ Specifications

Table 5.5. Summary of Microscale Generated Material Properties

<table>
<thead>
<tr>
<th>$V_f$</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
<th>$\nu_{12}$</th>
<th>$\nu_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room</td>
<td>80</td>
<td>186.77</td>
<td>12.31</td>
<td>10.26</td>
<td>4.43</td>
<td>0.31</td>
</tr>
<tr>
<td></td>
<td>73.3</td>
<td>172.15</td>
<td>12.09</td>
<td>8.93</td>
<td>4.32</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>37.5</td>
<td>92.24</td>
<td>9.96</td>
<td>4.61</td>
<td>3.46</td>
<td>0.36</td>
</tr>
<tr>
<td>Hot/Wet</td>
<td>80</td>
<td>167.81</td>
<td>10.78</td>
<td>10.15</td>
<td>3.80</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>73.3</td>
<td>154.2</td>
<td>10.58</td>
<td>8.83</td>
<td>3.73</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td>37.5</td>
<td>79.77</td>
<td>6.64</td>
<td>4.55</td>
<td>2.26</td>
<td>0.40</td>
</tr>
</tbody>
</table>

A local strain-width and stress-width analysis of the subcells is performed by extracting data at the center of the unit cell simulations along the $y_2$ direction to understand the effect of environmental conditions on the transverse tension response. The stress-width and strain-width results are plotted for unit cell strains of 0.15% and 0.55%, and are
presented in Figure 5.11. The analysis indicates that large stress and strain gradients exist at the fiber/polymer matrix interface for the unit cells with large $V_f$ values; smaller gradients are observed for the unit cells with small fiber volume fraction. These trends are due to the varying sizes of the polymer subcells which surround the carbon fiber, where the unit cell geometries with larger polymer subcells have increased compliance at the interphase. A comparison of the different conditions demonstrates that the hot/wet condition increases the compliance at the interface, as a result, less stress is transferred to the fiber subcells.
5.3.2. Macroscale Simulation Results

The macroscale stress-strain results for the room and hot/wet conditions of the axial tension models are presented in Figure 5.12 and Figure 5.13, respectively. Each level of element refinement is shown in these figures and the axial tension data from the experiments in Chapter 4 are also plotted for comparison. Good correlation is observed between the simulated and experimental responses up to the average PEL strain observed in the experiments, which was 1.98% for the room condition and 1.7% for the hot/wet condition. The principal strain contours from the axial tension simulations are nonuniform but strain concentrations are not prevalent along the edges of the models (Figure 5.14). As a result, small material features are not critical and the simulated stress-strain responses for each element refinement overlap, which signifies that convergence occurs with the coarse
meshed model (5,775 elements). Table 5.6 compares the elastic modulus calculated from each refined axial tension model with the average modulus measured from experiments.

Figure 5.12. Simulated and Experimental Stress-Strain Plots for the Axial Tension Loading under Room Condition

Figure 5.13. Simulated and Experimental Stress-Strain Plots for the Axial Tension Loading under Hot/Wet Condition
The room and hot/wet transverse tension data from the refined models and experiments are also plotted in Figure 5.15(a) and Figure 5.16(a), respectively. Unlike the axial tension model, the transverse tension simulations show that convergence is dependent on the mesh refinement of the models. This dependency is due to the intricate material
features, including edge effects, which are resolved only with finer meshes. The results from the finest mesh (90,720 elements) converge to the experimental data for both the room and hot/wet conditions. The room and hot/wet conditions simulation results using this mesh size are presented in Figure 5.15(b) and Figure 5.16(b), respectively, for the models with and without undulation. The elastic modulus is calculated for each refined transverse model and displayed in Table 5.7. The results for the model without tow undulation exhibit a larger stiffness than the results with tow undulation. This observation is not physically meaningful and can be attributed to the 2D nature of the material vectors defined for the model without undulating tows. For the model without tow undulation, the material vectors are defined on the xy-plane and only consider the braid angle of the material. Therefore, the material stiffness applied to the elements is also restricted to the xy-plane which leads to larger, unrealistic stiffness values. For the model with both tow undulation and braid angles, the material vectors have a z-direction component; thereby, a portion of the tow’s axial stiffness is redistributed to the z-direction which increases the element stiffness in the z-direction and decreases the stiffness values in the x- and y-directions. Hence, the architecture of the triaxial material is better preserved and a realistic transverse response is obtained.
Figure 5.15. Stress-Strain Results for the Transverse Tension Model at the Room Condition Comparing (a) the Simulated and Experimental Data and (b) the Plots of the Model with and without Undulation.

Figure 5.16. Stress-Strain Results for the Transverse Tension Model at the Hot/Wet Condition Comparing (a) the Simulated and Experimental Data and (b) the Plots of the Model with and without Undulation.
Table 5.7. Transverse Tension Elastic Moduli

<table>
<thead>
<tr>
<th></th>
<th>Room</th>
<th>Hot/Wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation – 5,670 elements</td>
<td>47.63 GPa</td>
<td>46.89 GPa</td>
</tr>
<tr>
<td>Simulation – 22,680 elements</td>
<td>45.55 GPa</td>
<td>43.85 GPa</td>
</tr>
<tr>
<td>Simulation – 90,720 elements</td>
<td>41.69 GPa</td>
<td>40.43 GPa</td>
</tr>
<tr>
<td>Experiment</td>
<td>42.10 ± 2.19 GPa</td>
<td>37.19 ± 0.83 GPa</td>
</tr>
</tbody>
</table>

In addition to the stress-strain responses, the effect of undulation is also observed in the local features in the principal strain field. The principal strain contours for the room and hot/wet condition of the transverse tension models are depicted in Figure 5.17 and Figure 5.18, respectively. The contour images are extracted from a simulation stage corresponding to the PEL strain for each condition, which is 0.96% for the room condition and 0.76% for the hot/wet condition. Additionally, the results from the transverse tension model without tow undulation are also shown (Figure 5.17c and Figure 5.18c). The principal strain contours from the simulations with tow undulation show similar intensities and patterns as those obtained from the DIC measurements of the experiments. However, the results of the model without tow undulation show that the features cannot be clearly resolved at the PEL due to the lack of out-of-plane properties, and these features only appear at later stages of the simulation. A direct measurement of the strain concentrations at the edges of the specimen demonstrates that the pattern is repeated every 17.8 mm according to the experimental data and 18.1 mm using the simulation results, which is further validation that the physical architecture of the material is adequately represented.
Figure 5.17. Comparison of Principal Strain Contours from Transverse Tension Experimental and Simulation Data at the Room Condition

(a) Experiment  
(b) Simulation with Undulation  
(c) Simulation without Undulation

Figure 5.18. Comparison of Principal Strain Contours from Transverse Tension Experimental and Simulation Data at the Hot/Wet Condition

(a) Experiment  
(b) Simulation with Undulation  
(c) Simulation without Undulation
5.4. Chapter Summary

The multiscale framework provided in this chapter consists of high fidelity micromechanics as well as a mesoscale and macroscale which are modeled and simulated using the LS-DYNA software package. The high fidelity generalized method of cells is applied to obtain microscale unit cell results and this micromechanical theory is detailed in Chapter 3. Temperature and moisture terms are used in the subcell constitutive laws so the higher order displacement field of the micromechanical theory accurately captures the effects of the mismatch in thermal and moisture expansion. The viscoplastic theory, described in Chapters 2 and 3, is utilized in the microscale polymer subcells in order to determine the appropriate elastic range for each type of microscale geometry and loading. Three microscale geometries are constructed based on the different $V_f$ specifications of the mesoscale subcells, and each geometry is simulated using the room and hot/wet conditions. The mesoscale model discretizes the RUC of the triaxial material into five subcells in order to incorporate the axial tows, braid angles, and tow undulation. The tow orientations are defined using 3D material vectors in the material keywords of the LS-DYNA software. The coarse mesh of the macroscale model incorporates the mesoscale subcells as finite elements and repeats the mesoscale structure to create a six ply, macroscale specimen model. The following results and conclusions are observed for the micro- and macroscale simulations:

1. The microscale simulations demonstrate that the unit cell geometries with larger $V_f$ values yield stiffer responses for the axial tension, transverse tension, and in-plane shear loadings; and the mismatch in thermal and moisture properties, due to hot/wet condition, causes a reduction in each response.
2. The local strain-width and stress-width analysis of the microscale, transverse tension simulations demonstrate that the larger $V_f$ geometries increase the stress and strain gradients across the fiber/polymer interface of the unit cells.

3. A comparison of the local strain-width and stress-width analyses show that the hot/wet condition increases the compliance at the interface which cause less stress to be distributed to the fiber subcells.

4. The results for the macroscale simulations of the axial tension and transverse tension specimens confirm that the models correlate well with the behavior observed in the experiments discussed in Chapter 4.

5. The principal strain contours from the macroscale simulations match the intensities and patterns of the contours obtained from experiments and demonstrate that the incorporation of tow undulation in the transverse tension models is essential for fully resolving these strain features.
6. CONTRIBUTIONS AND FUTURE WORK

6.1. Contributions

The primary objective of the research presented in this dissertation was to investigate the effect of material variability and environmental conditions on PMC behavior and failure. This objective was achieved by performing testing, characterization studies, and modeling of different composites. Four major contributions were achieved by this work: i) A stochastic micromechanics framework was developed, with progressive damage and multiscale failure theories, to investigate the effect of variability on the modeled composite response, ii) A high fidelity micromechanics technique was adapted by incorporating progressive damage and multiscale failure criteria to study the influence of shear coupling and various interphase properties, iii) Experiments were performed on triaxial braided PMCs to characterize the effect of various environmental conditions on the mechanical properties, damage, and failure of the material, and iv) A multiscale modeling framework was created to account for environmental conditions as well as 3D material architecture, and to validate the response of macroscale specimen models. The characterization data and modeling frameworks developed through this research illustrate the severity of material variability and environmental conditions on composites. This research represents substantial progress towards the development of a stochastic multiscale framework for modeling complex PMC architectures.
6.2. Future Work

While the research shown in this dissertation improves the fidelity of PMC modeling and contributes to the further understanding of composite behavior and failure, developments and additional testing can be done to improve the effectiveness of the modeling framework and to continue advancing the understanding of the composite material. The following future work topics are essential for advancing this research:

1. The research presented in Chapter 2 provides a stochastic multiscale modeling framework capable of accounting for material variability. The characterization of local and spatial $V_f$ variability of the composite microstructure is applied to an ordered composite unit cell to generate stochastic stress-strain plots. The characterization data could be used to generate stochastic representative volume elements (SRVE) consisting of multiple fibers at the microscale instead of using an ordered unit cell. The microscale SRVE, combined with a high fidelity micromechanics theory for shear coupling purposes, would improve the representation of the physical material structure and the prediction for progressive damage and failure. The fibers proximity to each other could be varied causing the formation of high stress concentrations which would lead to local damage and failure variability in the composite model. A foreseeable challenge in combining HFGMC with an SRVE would be a significant increase in the number of subcells in the model which would increase the computational cost. One way to overcome this difficulty would be the mapping of the subcells to a parametrical coordinate system. This mapping would allow a subcell to be any type of quadrilateral and could be used to optimize the number of subcells in the model. By better capturing
the stochastic, local failure, the modeling framework could be extended to simulate fatigue and fracture loadings.

2. In addition to incorporating microstructure and material property variability, the stochastic micromechanics framework could be extended to include epistemic variability. Epistemic variability, also called the model or physics variability, is the uncertainty related to the model’s formulation and laws. Several aspects of the current stochastic modeling framework could be modified to integrate epistemic variability including the viscoplastic law, progressive damage theory, and multiscale failure criteria. Using the macroscale failure theory, for example, the stochastic framework currently only applies the modified Hashin failure criteria. The Tsai-Wu, Tsai-Hill, Puck, and any number of failure theories could be applied to the stochastic framework by using the LHS technique to generate a random number which would be unique to each failure theory. Therefore, the stochastic macroscale failure of the model would have a larger variance and would better capture the material response.

3. For the triaxial braid composite characterization in Chapter 4, the effect of room and high temperature were studied as well as humidity. While these conditions were based on realistic environments induced on the aircraft composite components, the knowledge of composite behavior and failure could be expanded by performing the testing at other interval high temperatures as well as cold temperatures. Additionally, performing other tests such as fatigue or impact would expand the data and knowledge base of the triaxial braided composite which would increase the applicability of the material.
4. The multiscale modeling of the triaxial braid composite in this work is deterministic using average values for the constituent properties and orientation angles of the micromechanics simulations. This model could be enhanced by adding geometry and orientation variability to the mesoscale. The tow undulation and braid angle could be characterized to provide a statistical distribution of material properties for the micromechanics simulations. While some level of through thickness variability is achieved via the subcell shift technique of the mesoscale RUC, additional through-thickness variability could be introduced by randomly shifting the mesoscale subcells. In addition, the physical triaxial architecture could be directly reproduced using 3D microstructural reconstruction techniques. The data generated from this reconstruction would provide accurate measurements for improved subcell dimensions and geometry, and it could also be used to explicitly model the fiber tows via FEA models.
REFERENCES


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