Integration of micromechanical and probabilistic analysis models of nanocomposites

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A Thesis

entitled

Integration of Micromechanical and Probabilistic Analysis Models of
Nanocomposites

by

Srikanth Pilla

Submitted as partial fulfillment of the requirements for
the Master of Science in Mechanical Engineering

Advisor: Dr. Efstratios Nikolaidis

Graduate School

The University of Toledo

December 2005
The University of Toledo

College of Engineering

I HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER MY SUPERVISION BY Srikanth Pilla

ENTITLED Integration of Micromechanical and Probabilistic Analysis Models of Nanocomposites

BE ACCEPTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF Master of Science in Mechanical Engineering

Thesis Advisor: Dr. Efstratios Nikolaidis

Recommendation concurred by

Dr. Arunan Nadarajah

Dr. Lesley Berhan

Committee

On Final Examination

Dean, College of Engineering
An abstract of
Integration of Micromechanical and Probabilistic Analysis Models of Nanocomposites

Srikanth Pilla

Submitted as partial fulfillment of the requirements for
the Master of Science in Mechanical Engineering

The University of Toledo
December 2005

Carbon nanofiber/nanotube reinforced composites show great potential as a replacement for conventional composite materials because of their exceptional properties. Experimental results demonstrate that substantial improvements in the mechanical behavior of a nano-structured composite can be attained using small amounts of carbon nanofibers/nanotubes as reinforcing phase. To date many researchers have theoretically predicted the effective behavior of conventional composites and nanocomposites using traditional methods (for example using Mori-Tanaka or Halpin-Tsai models). The effect of the interface between the nanofibers/nanotubes and the matrix has also been investigated. There is uncertainty in the value of the modulus of the reinforcement in nanocomposites because it is difficult to measure the modulus. Moreover there is variability in the matrix and interface moduli. Therefore, it is important to study the effect
of uncertainty and variability in the properties of the phase materials on the properties of nanocomposite. A large amount of work has been done on modeling uncertainty and variability in conventional materials (e.g., aluminum, steel or long fiber composites) and on predicting the probability distribution of the performance characteristics of structures made of these materials. However, an integrated tool is needed for probabilistic analysis of structures made of carbon nanofiber/nanotube composites.

In this thesis, existing models for stiffness analysis of conventional composites and nanocomposites have been modified and integrated with tools for deterministic and probabilistic analysis of structures. A two-step model has been developed for determining deterministically the stiffness of nanocomposite materials considering the effect of the interface between the reinforcement and the matrix. A methodology consisting of the above two-step model, deterministic analysis of plates and probabilistic analysis of structures has also been developed and demonstrated. It is shown that it is important to consider the interface between the reinforcement and polymer matrix and the variability and uncertainty in the properties of the phase materials of a nanocomposite.
For my parents, Mohan and Padma

Their constant support and encouragement has made this thesis possible
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CHAPTER 1. INTRODUCTION

1.1. BACKGROUND AND MOTIVATION

Carbon nanofibers (CNFs) and carbon nanotubes (CNTs), which have been discovered in 1980s and 1990s respectively, have attracted considerable attention because of their outstanding physical properties. In addition to their small size, CNTs/CNFs are half as dense as aluminum, have high tensile strength, high current carrying capacity, and transmit heat twice as well as pure diamond [12]. Due to the advantages that CNTs/CNFs offer in terms of size and properties, they are used in a wide variety of applications, such as chemical and genetic probes, field emission tips, mechanical memory, ultra fine sensors, hydrogen and ion storage, scanning probe microscope tips, and structural components [12].

Composites made of CNTs/CNFs embedded in polymer matrix have attracted the attention of many researchers in recent years [11]. Reinforcing nano-structured material in polymers will provide better mechanical properties when compared to large scale reinforcements that are currently used for aerospace applications, such as carbon fibers.
[46]. In the development of nano-structured materials it is important to develop constitutive relationships that predict the bulk mechanical properties of these materials as a function of the properties of the polymer, reinforcement and their interface. These constitutive relationships will help in designing these materials before they are synthesized. The following paragraph illustrates the importance of developing an analytical model for predicting the properties of a composite from those of the constituent materials.

Figure 1-1 illustrates the importance of modeling in understanding the behavior of matter. As discussed in [48], first the material behavior is understood by observation via experiments. The experimental data is then carefully measured and models are developed for predicting the observed behavior under the corresponding conditions. The models are necessary to develop the theory. This theory is simulated to predict the behavior of the material analytically. The predicted behavior is then compared to observed behavior from experiments. This comparison serves to either validate the theory, or to provide a feedback loop to improve the theory using modeling data. Therefore, the development of a realistic theory of describing the structure and behavior of materials is highly dependent on accurate modeling and simulation techniques.
This study is part of an effort to develop and characterize a new carbon nanofiber composite in which complete functionalization – or bonding of the fiber and matrix – takes place, leading to enhanced and more predictable material properties. The responsibility of characterization is divided into several tasks, starting at the molecular level and moving to the macroscopic behavior of a structure via the micromechanical level. This thesis focuses on the development of a micromechanical model for predicting the stiffness of nanocomposite based on the properties of the individual phase materials.

The nano-structured materials studied in this thesis exhibit uncertainty in their properties due to variation found in the properties of base materials. It is very important to account for these uncertainties and variability while designing the material since they affect the behavior of material and the safety of structures made of this material. Therefore, it becomes important not only to develop a deterministic method for stiffness
prediction, but also to create a methodology that will quantify the effect of variations and the uncertainty in the properties of base materials on the properties of a nanocomposite.

1.2. LITERATURE REVIEW

There are vast resources of literature available on various aspects of this study, including stiffness prediction of conventional composites, stiffness prediction of nanocomposites, modeling of the interface between the nanofiber/nanotube and polymer matrix, and probabilistic analysis nanocomposites. Though an exhaustive treatment of the literature in these areas is beyond the scope of this study, an overview will be given.

1.2.1. CONVENTIONAL COMPOSITES

Fiber-reinforced composites are certainly one of the oldest and most widely used composite materials [4]. Their study and development have been largely carried out due to their vast structural potential. Much information on the formulation for stiffness of conventional fiber reinforced composites can be found in [4], [29], and [13].

1.2.2. NANOCOMPOSITES

Analysis of nanocomposites has been performed by many researchers recently. A review on experimental work done on polymer nanocomposites has been presented by Jordan et al. [30]. Qian et al. [37] and Andrews et al. [5] showed experimentally that small amounts of CNTs/CNFs substantially improve the properties of a composite material compared to the properties of the polymer matrix. This inference has been theoretically supported by Sheng et al. [41], Fisher [17] and Shi et al. [42]. These researchers used Mori-Tanaka method to model the behavior of nanocomposites. Mori-
Tanaka method predicts the average stress fields and overall effective stiffness of a composite with a non-dilute concentration of inclusions. Sheng et al. [41] did stiffness analysis of polymer/clay nanocomposites. They calculated the nanocomposite stiffness by considering multiscale micromechanical models accounting for the hierarchical morphology of the nanocomposite. They compared the results from their FEM model to Halpin-Tsai empirical method and Mori-Tanaka method. The strong dependence of the modulus of clay particles on the modulus of polymer has been a significant conclusion drawn by their study. Additionally, they compared FEM, Mori-Tanaka and Halpin-Tsai results with that of experimental ones and concluded that Halpin-Tsai predicts the nanocomposite to be too stiff while the FEM and Mori-Tanaka agree well with experiments. Out of the FEM and Mori-Tanaka, the former agrees best with experimental ones but the later provides a reasonably accurate analytical estimate for the nanocomposite modulus. Fisher [17] numerically predicted the waviness of nanofibers and incorporated this into Mori-Tanaka micromechanical method. Shi et al.’s work [42] is on the same lines of Fisher’s [17] but the nanofiber waviness prediction is done theoretically.

The bonding between the reinforcement and matrix affects significantly the mechanical and physical properties of nano-structured materials. For CNT/CNF reinforced composites, the high surface area of CNTs/CNFs creates a large interfacial region, which has properties different from the bulk matrix. A detailed study on interfaces of multicomponent materials has been done by Pukanszky [36]. Wagner et al.
[49], Lourie and Wagner [32], and Jia et al. [28] have studied the effect of interfacial bonding on the mechanical properties of CNT reinforced composites experimentally. Their studies have shown the effect of considering interface while analyzing a nanocomposite. The theoretical models used by Fisher [17] and Shi et al. [42] for predicting stiffness of nanocomposites assume perfect bonding and consequently yield an upper bound of the properties of the composite. The true value of the performance parameters can be considerably lower than those predicted by these models. Therefore, it is important to account for the degree of adhesion of the reinforcement to the matrix theoretically to improve the accuracy of a micromechanics model. Shi et al. [43] have modified their approach for stiffness prediction of nanocomposites [42] to include the effect of interface. They considered the interface as a third phase (an inclusion with different modulus than that of the nanotube) and used multiphase Mori-Tanaka micromechanical method to estimate the stiffness of the composite. They cited [8] as support for the assumption that the above multiphase model can describe the effect of the interface. Although, the results of Shi et al.’s approach are plausible, the assumption that the composite consists of the nanotube and the interface dispersed randomly in the matrix has not been justified adequately in the author’s opinion. Odegard et al [34] developed a model for analyzing the interface effect in nanocomposites, but their model considers the reinforcement’s shape to be spherical in geometry. When the author of this thesis modified this model for cylindrical reinforcements and tested it for unidirectional composites he did not obtain satisfactory results. Specifically, although, the variation in the Young’s modulus of the composite with the volume fraction of the reinforcement seemed reasonable, very little difference was found in the longitudinal and
transverse moduli. This result is counterintuitive, because for unidirectional composites, the longitudinal modulus should be much higher than the transverse modulus. Therefore, the author of this thesis believes that, although the model presented by Odegard et al. considers the physics of the problem, it doesn’t apply for cylindrical CNTs/CNFs.

1.2.3. PROBABILISTIC AND RELIABILITY ANALYSIS OF NANOCOMPOSITES

In engineering problems uncertainties can be classified as random and epistemic. Random uncertainty, or variability, refers to inherent randomness in natural phenomena or processes. Epistemic uncertainty is due lack of knowledge. The latter is also called reducible uncertainty because collecting data can reduce this type of uncertainty. Random uncertainty is sometimes referred to as irreducible uncertainty, because acquiring knowledge does not reduce the inherent uncertainty. Probabilistic analysis accounts for both variability and epistemic uncertainty.

Due to its nano structure, the modulus of the nanotubes/nanofibers cannot be estimated accurately. As a result the modulus is specified in terms of upper and lower bounds. Also, there is uncertainty in the modulus of the matrix and the interface between the nanotubes/nanofibers and the matrix. These uncertainties are important because of their magnitude. Hence it is important to account for the variability and uncertainties of the moduli of constituent materials of nanocomposite using probabilistic analysis. Many researchers, cited in [21], developed methods for probabilistic analysis and reliability analysis of conventional composites. Thostenson and Chou [47] used probabilistic models to account for the distribution of the diameters of CNT/CNFs. Hammitt [21] presented a methodology for reliability analysis of nanocomposite structures. However;
there is no literature in the public domain on probabilistic analysis of nanocomposites and of structures made of nanocomposites that accounts for the variability and uncertainty in the moduli of the constituent materials.

1.3. SCOPE AND OBJECTIVES

As mentioned in Section 1.2, there has been significant work in the areas of stiffness analysis of conventional composites and nanocomposites, and in reliability methods. What is lacking, however, is an integrated methodology for deterministic and probabilistic analysis of conventional and nanocomposite materials and structures made of these materials. The deterministic analysis could determine the stiffness of conventional and nanocomposite materials. The stiffness of a nanocomposite is predicted by considering the effect of interface between CNT/CNF and polymer matrix. The probabilistic analysis could determine the PDF of the modulus of a nanocomposite and the sensitivity of the nanocomposite modulus to the moduli of the phase materials. These parameters include those variables that can be controlled by the designer (e.g. the moduli of nanofiber/nanotube), and statistical parameters (e.g. the mean and standard deviation of the moduli of the polymer matrix and interface).

The objective of this study is to integrate a model for predicting the stiffness of conventional composites and nano composites (with and without considering the interface) and another model for probabilistic analysis with models for failure and reliability analysis.

For conventional composites, either the material properties of the orthotropic lamina, and the stacking sequence, can be supplied directly as input to the methodology, or the composition of the composite can be given along with properties of the matrix and fiber.
For nanocomposites, the properties of the phase materials (CNT/CNF, matrix and interface) are to be supplied along with respective volume fractions. The phase material properties can be estimated from experiments or from molecular dynamics models. Output of the methodology includes the stiffness matrix of conventional or nanocomposite and the mean and standard deviation of the modulus of nanocomposite. For the failure and reliability analysis methodology, the output includes the load-deflection data for a plate under axial or transverse loading, probability of failure by the important failure modes, and sensitivity of the failure probability of these failure modes to variation in each of the random input variables.

In the present study, the nanofibers/nanotubes are assumed to be straight and agglomeration is not considered, so the nanocomposite is assumed to be macroscopically homogeneous. In the encapsulated inclusion interface model, the interface is assumed to surround the CNT/CNF only on the circumference but not on the circular ends.

1.4. CONTRIBUTIONS OF THIS STUDY

1. The first contribution of this study is an integration of four models which are shown in Figure 1-2 and are explained below:

   a. A model for predicting the stiffness of conventional and nanocomposites (with and without considering the CNT/CNF-matrix interface)
   b. A model for probabilistic analysis of nanocomposites
   c. A model for predicting the strength and for performing failure analysis of conventional composites and nanocomposites
   d. A model for reliability analysis of conventional and nanocomposites
2. The second contribution is a development of an encapsulated inclusion model to account for the interface between the nanofiber/nanotube and the polymer matrix. This encapsulated model can be used to predict the stiffness of the nanocomposite. This model is an extension of model presented by Shi et al. [43].

3. The third contribution of this study is the development of tools for probabilistic analysis of nanocomposites. This analysis in addition to accounting for the variability and uncertainty in phase material properties performs sensitivity analysis to identify the properties whose variation has the most significant impact on the stiffness of nanocomposite material, providing valuable information about those properties that must be controlled most carefully.

A custom Fortran 90 code was developed by the author for the stiffness of conventional and nanocomposites and probabilistic analysis for nanocomposites, and existing in-house codes were utilized for the strength and reliability models. The in-house codes provide the user with more flexibility than commercial codes and facilitate the exchange of information between the models (Figure 1-2).
This study also lays a foundation for future work on modeling spatial variation of material properties. The in-house code can be modified to reflect new information about the behavior of nanocomposites. The method could also be used to analyze continuous-fiber composite laminates where a carbon nanofiber composite is used as the matrix material, and conventional carbon fibers are added to further enhance structural strength and performance.

1.5. OUTLINE OF THESIS

First this study presents a model for predicting the stiffness of conventional composites with unidirectional fibers and short randomly oriented fibers. Then the
mechanics of lamina and laminate is presented. These are based on well established theories presented in Agarwal and Broutman [4], Jones [29] and Daniel [13].

Chapter 4 focuses on micromechanical modeling of nanofiber/nanotube composites based on Mori-Tanaka [33] theory without taking into consideration the interface between the nanofibers/nanotubes and matrix. A numerical example has been presented that integrates Mori-Tanaka method and the failure and reliability analysis model developed by Hammitt [21] to give load-deflection history of a structure made of nanocomposite materials. Hammitt developed the failure and reliability model based on well established finite element and reliability analysis tools.

Chapter 5 presents a model for predicting the stiffness of nanocomposites by considering the reinforcement/matrix interface. A modified two-step approach that uses two concentric cylinders (henceforth called inclusion) encapsulated in the matrix is developed by the author based on the theories presented by Whitney and Riley [51], Agarwal and Broutman [4] and Mori and Tanaka [33]. It is a continuum-based constitutive model for nanocomposites. The model assumes that all three layers (CNT/CNF, interface and matrix) are continuous and perfectly bonded to each other. It further assumes that the inclusion consists of the nanofiber/nanotube inserted in a hollow cylinder representing the interface is embedded into the matrix. This model computes the elastic modulus of nanocomposite in two steps. First, a mechanics approach [51] is used to compute the properties of the inclusion whose physical structure is similar to the three-phase unit cell model presented in [43]. In the second step, Mori-Tanaka [33] model is employed to estimate the elastic properties of the composite from those of the inclusion and matrix. Numerical examples demonstrating the developed approach are presented.
Chapter 6 details the methodology for probabilistic analysis of nanocomposites. The methodology consists of a probabilistic model for estimation of the probability density function (PDF) of the modulus of a nanocomposite given the PDF’s of the properties of the constituent materials. This is done using Monte Carlo simulation [38]. This PDF is used in the tool for reliability analysis for nanocomposites developed by Hammitt [21]. Numerical examples for both the analyses are presented.

Finally, the study is summarized. Then the main conclusions of this study and recommendations for improvements of the developed tools are presented.
CHAPTER 2. MECHANICS OF UNIDIRECTIONAL AND SHORT FIBER COMPOSITES

2.1. INTRODUCTION

Fiber-reinforced composites are certainly one of the oldest and most widely used composite materials [4]. Their study and development have been largely carried out due to their vast structural potential. The majority of the structural elements or laminates made of fibrous composites consist of several distinct layers of unidirectional laminae. Each lamina is made of the same constituent materials (matrix and fiber). But an individual layer may differ from other layer in:

1. volume fraction of the constituent materials,
2. type of reinforcement used such as continuous or discontinuous fibers,
3. orientation of fibers with respect to a common reference axis.

Additionally there are hybrid laminates consisting of layers having different fibers and/or matrix material. Thus the directional properties of the individual layers may be quite different from each other. Analysis and design of any laminate would require a complete knowledge of the properties of individual layers. A single-layer composite, therefore, represents a basic building block for laminate constructions. This chapter focuses on predicting the elastic properties of unidirectional and short fiber composites. The methods
presented in this chapter are already available in text books and papers. The reason of presenting them in this study is that they are fundamental for the development of methods presented in chapters 4 and 5.

2.1.1. TERMINOLOGY

A unidirectional composite consists of parallel fibers embedded in a matrix. Several unidirectional layers can be stacked in a specified sequence of orientation to fabricate a laminate that will meet design strength and stiffness requirements. Each layer of a unidirectional composite may be referred to as simply a layer, ply, or lamina.

A unidirectional composite is shown in Figure 2-1. The direction parallel to the fibers is generally called the longitudinal direction (axis 1). The direction perpendicular to the fibers is called the transverse direction (any direction in the 2-3 plane). These axes are also referred to as the material axes of the ply.
The lamina in Figure 2-1 has only one fiber through the ply thickness. In practice, this may be only true for large-diameter fibers. Plies with short-diameter fibers have several fibers through the actually ply thickness. The fibers are randomly distributed throughout the cross section and may be in contact with each other in some locations. This type of fiber distribution in the lamina is typical of several fiber-matrix systems.

Because of the structure of the composite, a unidirectional composite shows different properties in the longitudinal and transverse directions. Thus, the unidirectional composites are orthotropic with the axes 1, 2, and 3 as the axes of symmetry (Figure 2-1). A unidirectional composite has the strongest properties in the longitudinal direction. Because of the random fiber distribution in the cross section, material behavior in the
other two directions (2, 3) is nearly identical. Therefore, a unidirectional composite or ply can be considered to be transversely isotropic; that is, it is isotropic in the 2-3 plane.

### 2.1.2. VOLUME AND WEIGHT FRACTIONS

The properties of composites are mainly determined by the relative proportions of the matrix and reinforcing materials. The relative proportions can be given as the weight fractions or the volume fractions. The weight fractions are usually obtained during fabrication or by one of the experimental methods after fabrication. However, in theoretical analysis of composite materials, the volume fractions are exclusively used. Thus expressions for conversion between the weight fractions and volume fractions are determined. These expressions are derived for a two-phase material and then generalized to a multiphase material.

Consider a volume $v_c$ of a composite material that consists of volume $v_f$ of the fibers and volume $v_m$ of the matrix material. Let $w_c, w_f$ and $w_m$ represent weights of composite material, fibers and matrix respectively. (Throughout this thesis, subscripts c, f, and m are consistently used to represent the composite material, fibers, and the matrix material, respectively.) Let the volume fraction and weight fraction be denoted by the capital letters $V$ and $W$, respectively. The volume fractions and weight fractions are defined as follows:

$$v_c = v_f + v_m \quad \text{(2-1)}$$

$$V_f = \frac{v_f}{v_c}, \quad V_m = \frac{v_m}{v_c} \quad \text{(2-2)}$$
\[ w_c = w_f + w_m \]  
\text{2-3}

and

\[ W_f = \frac{W_f}{w_c}, \quad W_m = \frac{W_m}{w_c} \]  
\text{2-4}

We need the density of the composite material, \( \rho_c \), to establish conversion relations between the weight fractions and the volume fractions. The density of the composite material can be easily obtained in the terms of the densities of the fiber and matrix and their volume fractions or weight fractions. Rewriting Eq. 2-3 in terms of densities and volume yields

\[ \rho_c v_c = \rho_f v_f + \rho_m v_m \]  
\text{2-5}

Diving both sides of Eq. 2-5 by \( v_c \) and substituting the definition for the volume fractions from Eq. 2-2 yields

\[ \rho_c = \rho_f \frac{v_f}{v_c} + \rho_m \frac{v_m}{v_c} \]  
\text{2-6}

\[ \rho_c = \rho_f V_f + \rho_m V_m \]  
\text{2-7}

The density of composite materials in terms of weight fractions is obtained by similar manipulations in Eq. 2-1 as

\[ \rho_c = \frac{1}{(W_f / \rho_f) + (W_m / \rho_m)} \]  
\text{2-8}
Now the conversion between the weight fraction and volume fraction can be obtained by considering the definition of weight fraction and replacing in it the weights by the products of density and volume as follows:

\[
W_f = \frac{w_f}{w_c} = \frac{\rho_f v_f}{\rho_c v_c} = \frac{\rho_f}{\rho_c} V_f
\]

\[
W_f = \frac{\rho_f}{\rho_c} V_f
\]  

2-9

\[
W_m = \frac{\rho_m}{\rho_c} V_m
\]

The inverse relations can be similarly obtained from Eq. 2-1 - 2-4 or 2-9 by multiplying both sides of the equation by an appropriate ratio of densities. The inverse relations are:

\[
V_f = \frac{\rho_c}{\rho_f} W_f
\]  

2-10

\[
V_m = \frac{\rho_c}{\rho_m} W_m
\]

Equations 2-6 - 2-10 have been derived for a composite material with only two constituents but can be generalized for an arbitrary number of constituents. The generalized equations are:

\[
\rho_c = \sum_{i=1}^{n} \rho_i V_i
\]

\[
\rho_c = \frac{1}{\sum_{i=1}^{n} (W_i / \rho_i)}
\]  

2-11
The composite density calculated theoretically from weight fractions using Eq. 2-9 may not always be in agreement with the experimentally determined density because of the presence of voids in the composite. The difference in densities indicates the void content. The volume fraction of the voids in terms of the theoretical and experimental composite densities is given in Eq. 2-12; however, a proof of this condition is beyond the scope of this thesis.

\[ V_v = \frac{\rho_{ct} - \rho_{ce}}{\rho_{ct}} \]

- \( V_v \) – Volume fraction of voids 2-12
- \( \rho_{ct} \) – Theoretical composite density
- \( \rho_{ce} \) – Experimental composite density

2.2. LONGITUDINAL STIFFNESS

The properties of a composite material depend on the properties of its constituent materials (fiber and matrix) and their distribution and physical and chemical interactions. The properties of composites can be determined through simple and direct experimental measurements. However, one set of experimental measurements determines the properties of a fixed fiber-matrix system produced by a single fabrication process. Additional measurements are required when there is a change in the system variables such as the relative volumes of the constituents, constituent properties, and fabrication
process. Thus experiments may become time consuming and cost prohibitive. Theoretical and semi empirical methods of determining composite properties can be used to predict the effects of a large number of system variables. All of these methods may not be reliable for component design purposes. They might present difficulty in selecting a representative but tractable mathematical model for some properties such as the transverse properties of unidirectional composites. However, the mathematical model for studying the longitudinal properties of a unidirectional composite is quite accurate. Properties related to loading in the fiber direction are dominated by the fibers that are usually stronger and stiffer.

2.2.1. INITIAL BEHAVIOR

Consider a unidirectional composite with uniform properties of fiber and matrix. The fibers are assumed to be parallel throughout the composite (Figure 2-2). It may be further assumed that a perfect bonding exists between the fibers and the matrix so that no slippage can occur at the interface. As a result, the strains experienced by the fiber, matrix, and the composite are equal

\[ \varepsilon_f = \varepsilon_m = \varepsilon_c \]
Figure 2-2 A unidirectional composite model for predicting longitudinal modulus (adapted from [4])

For this model the load \((P_c)\) carried by the composite is shared between the fibers \((P_f)\) and the matrix \((P_m)\) so that

\[ P_c = P_f + P_m \]  \hspace{1cm} 2-14

The loads \(P_c, P_f,\) and \(P_m\) carried by the composite, the fibers, and the matrix, respectively, may be written as follows in terms of stresses \(\sigma_c, \sigma_f,\) and \(\sigma_m\) experienced by them and their corresponding cross-sectional areas \(A_c, A_f,\) and \(A_m.\) Thus

\[ P_c = \sigma_c A_c = \sigma_f A_f + \sigma_m A_m \]  \hspace{1cm} 2-15

or,

\[ \sigma_c = \sigma_f \frac{A_f}{A_c} + \sigma_m \frac{A_m}{A_c} \]  \hspace{1cm} 2-16

But for composites with parallel fibers, the volume fractions are equal to the area fractions such that
\[ V_f = \frac{A_f}{A_c}, V_m = \frac{A_m}{A_c} \]  \hspace{1cm} 2-17

Thus

\[ \sigma_c = \sigma_f V_f + \sigma_m V_m \]  \hspace{1cm} 2-18

Now Eq. 2-18 can be differentiated with respect to strain, which is the same for the composite, the fibers, and the matrix. The differentiation yields

\[ \frac{d\sigma_c}{d\epsilon} = \frac{d\sigma_f}{d\epsilon} V_f + \frac{d\sigma_m}{d\epsilon} V_m \]  \hspace{1cm} 2-19

where \((d\sigma / d\epsilon)\) represents the slope of the corresponding stress-strain diagrams at the given strain. If the stress-strain curves of the materials are linear, the slopes, \((d\sigma / d\epsilon)\), are constants and can be replaced by the corresponding elastic modulus in Eq. 2-19.

\[ E_c = E_f V_f + E_m V_m \]  \hspace{1cm} 2-20

The longitudinal modulus of a unidirectional composite as predicted by Eq. 2-20 has been plotted in Figure 2-3 as a function of the fiber volume fraction.
Thus Equations (2-18)-(2-20) indicate that the contributions of the fibers and the matrix to the average composite properties are proportional to their volume fractions. Such a relationship is called *rule of mixtures*. Equations 2-18 and 2-20 can be generalized as

\[ \sigma_c = \sum_{i=1}^{n} \sigma_i V_i \]  
\[ 2-21 \]

\[ E_c = \sum_{i=1}^{n} E_i V_i \]  
\[ 2-22 \]
2.3. TRANSVERSE STIFFNESS

In the case of transverse normal loading, the state of stress in the matrix surrounding the fibers is complex and more affected by interaction from neighboring fibers [13]. The transverse modulus is a matrix-dominated property and it is sensitive to the local state of stress.

2.3.1. CONSTANT-STRESS MODEL

A mathematical model similar to the one constructed in Section 2.2 can be constructed to study the transverse properties of composites. The fibers are assumed to be uniform in properties, diameter, continuous and parallel throughout the composite. The composite is stressed in the direction perpendicular to the parallel fibers that is the transverse direction. The model for predicting the transverse properties of a unidirectional composite may be considered to be made up of layers representing fibers and matrix material as shown in Figure 2-4. Each layer of fiber and matrix is perpendicular to the direction of loading and has the same area on which the load acts. Hence each layer will carry the same load and experience equal stress, that is

\[ \sigma_f = \sigma_m = \sigma_c \]  

2-23
The thickness of each layer is assumed to be same so that the cumulative thickness of fiber layers and matrix layers will be proportional to their respective volume fractions. In this case the sum of elongation of constituent materials that is fiber ($\delta_f$) and matrix ($\delta_m$) is equal to the composite elongation ($\delta_c$) in the direction of the load,

$$\delta_c = \delta_f + \delta_m$$  \hspace{1cm}  \text{(2-24)}

The elongation in the material can be written as the product of the strain and its cumulative thickness,

$$\delta_c = \varepsilon_c t_c$$

$$\delta_f = \varepsilon_f t_f$$  \hspace{1cm}  \text{(2-25)}

$$\delta_m = \varepsilon_m t_m$$

Substituting Eq. 2-25 in Eq. 2-24 gives

$$\varepsilon_c t_c = \varepsilon_f t_f + \varepsilon_m t_m$$  \hspace{1cm}  \text{(2-26)}
Dividing both sides of Eq. 2-26 by $t_c$ and substituting volume fraction for thickness yields

$$\varepsilon_c = \varepsilon_f \frac{t_f}{t_c} + \varepsilon_m \frac{t_m}{t_c} \quad 2-27$$

$$\varepsilon_c = \varepsilon_f V_f + \varepsilon_m V_m$$

If the fibers and the matrix are now assumed to deform elastically, the strain can be written in terms of the corresponding stress and the elastic modulus as follows:

$$\frac{\sigma_c}{E_c} = \frac{\sigma_f}{E_f} V_f + \frac{\sigma_m}{E_m} V_m \quad 2-28$$

In view of Eq. 2-23, Eq. 2-28 can be simplified as

$$\frac{1}{E_c} = \frac{V_f}{E_f} + \frac{V_m}{E_m} \quad 2-29$$

The transverse modulus of a unidirectional composite as predicted by Eq. 2-29 has been plotted in Figure 2-5 as a function of the fiber volume fraction.
The transverse modulus of a composite with $n$ number of materials may be obtained by generalizing Eq. 2-29

$$E_c = \frac{1}{\sum_{i=1}^{n} \left( V_i / E_i \right)}$$ \hspace{1cm} 2-30

The constant-stress model described above is not mathematically vigorous [4]. In a real composite, the parallel fibers are dispersed randomly in the matrix material. Generally both the fibers and matrix are present at any section perpendicular to the load, especially at higher fiber volume fractions. Thus the load is shared between the fibers and the matrix, and the assumption that the stresses in the fiber and matrix are equal is
inaccurate. The assumption of equal stresses also results in a mismatch of strains in the loading direction at the fiber-matrix interface. Another inaccuracy arises due to the mismatch of Poisson ratios of the fibers and the matrix, which induces stresses in the fibers and matrix perpendicular to the load with no net resultant force on the composite in that direction. A mathematically rigorous solution with a complete match of displacements across the boundary between the fiber and the matrix is accomplished through the use of the theory of elasticity\(^1\) [4]. Although sufficient and useful information can be generated through a theory of elasticity approach, most of the results are in the form of curves and complicated equations, thus limiting their adoptability to design procedures [4]. For design purposes, it is often desirable to have simple and computationally fast procedures for estimating the properties of composite even though the estimates are only approximate. Thus Halpin-Tsai has developed some semi-empirical equations for predicting the transverse modulus of a composite.

2.3.2. HALPIN-TSAI MODEL

Halpin and Tsai [20] have developed simple and generalized semi-empirical equations to approximate the transverse properties of unidirectional composites. These equations are simple and can be easily used in the design process. Furthermore, the predictions of these equations are good enough as long as fiber volume fraction does not approach 1. The Halpin-Tsai equation for transverse composite modulus can be written as

\[
\frac{E_T}{E_m} = \frac{1 + \xi \eta V_f}{1 - \eta V_f}
\]

\[2-31\]

\(^1\) Theory of elasticity approaches are beyond the scope of this thesis
where

\[ \eta = \frac{\left( \frac{E_f}{E_m} \right)^{-1} - 1}{\left( \frac{E_f}{E_m} \right)^{+} + \xi} \]  \hspace{1cm} 2-32

\( \xi \) is a measure of reinforcement and depends on the fiber geometry, packing geometry, and loading conditions. The values of \( \xi \) can be obtained by substituting Eq. 2-31 in 2-32 and comparing it with exact elasticity solutions through curve-fitting techniques. According to Halpin and Tsai the value of \( \xi = 2 \) may be used for fibers with circular cross section. For rectangular cross-section fibers, \( \xi \) may be calculated as

\[ \xi = 2 \frac{a}{b} \]  \hspace{1cm} 2-33

where \( a/b \) is the rectangular cross-section aspect ratio with the dimension \( a \) taken in the direction of the loading.

Figure 2-6 shows the predictions of Halpin-Tsai equation for transverse composite modulus as a function of fiber volume fraction for different constituent modulus ratios. Halpin and Tsai [20] have demonstrated the accuracy of Eq. 2-31 by showing that the predictions of Eq. 2-31 agree well with some of the more exact solutions. A more thorough discussion on comparison of Hapin-Tsai equations with that of exact elasticity solution is presented in the original reference [20].
Halpin-Tsai equations are quite adequate to satisfy the practical requirements for the predictions of transverse modulus of composite, particularly as the variations in composite materials manufacturing processes always cause a variation in the composite moduli [29].

2.4. SHEAR MODULUS

The behavior of unidirectional composites under in-plane (longitudinal) shear loading is also dominated by the matrix properties and the local stress distributions [13].
2.4.1. CONSTANT-STRESS MODEL

The longitudinal shear modulus of a unidirectional composite can be predicted using the constant stress model used for transverse modulus in section 2.3.1. As shown in Figure 2-7, a unidirectional composite is subjected to shear loading. Shearing stresses on the fibers and the matrix are equal. Thus

\[ \tau_f = \tau_m = \tau_c \]

The total shear deformation of the composite \((\Delta_c)\) is the sum of the shear deformations of the fibers \((\Delta_f)\) and the matrix \((\Delta_m)\):

\[ \Delta_c = \Delta_f + \Delta_m \]

Figure 2-7 (a) A unidirectional composite model for predicting the shear modulus and (b) the shear deformations of the model shown for cumulative thickness of constituents (adapted from [4])

Recognizing that the shear deformation in each material can be written as the product of corresponding shear strain \((\gamma)\) and the cumulative thickness of the material:

\[ \Delta_c = \gamma_c t_c \]
\[ \Delta_f = \gamma_f t_f \]
\[ \Delta_m = \gamma_m t_m \]

Substituting Eq. 2-36 in Eq. 2-35 yields
\[ \gamma_c \Delta_c = \gamma_f t_f + \gamma_m t_m \quad 2-37 \]

Dividing both sides of Eq. 2-37 by \( t_c \) and substituting volume fraction for thickness yields
\[ \gamma_c = \gamma_f \frac{t_f}{t_c} + \gamma_m \frac{t_m}{t_c} \quad 2-38 \]
\[ \gamma_c = \gamma_f V_f + \gamma_m V_m \]

Recognizing that for the linear behavior of shear stress-shear strain of fibers and matrix, the shear strains in Eq. 2-38 can be replaced by the ratios of shear stress and appropriate shear modulus yields
\[ \frac{\tau_c}{G_{LT}} = \frac{\tau_f}{G_f} V_f + \frac{\tau_m}{G_m} V_m \quad 2-39 \]

where \( G_{LT} \) is the in-plane shear modulus of the composite, \( G_f \) and \( G_m \) are the shear modulus of the fibers and matrix, respectively.

In view of Eq. 2-34, Eq. 2-39 can be simplified as
\[ \frac{1}{G_{LT}} = \frac{V_f}{G_f} + \frac{V_m}{G_m} \quad 2-40 \]

or
As pointed in Section 2.3.1, this model for predicting shear modulus of unidirectional composite is not accurate. The approach tends to underestimate the in-plane shear modulus [13]. Hence Halpin and Tsai [20] have developed simple equations to approximate the results of more exact micro mechanics analysis.

2.4.2. HALPIN-TSAI MODEL

The Halpin-Tsai equations for in-plane shear modulus of a unidirectional composite can be written as

\[
G_{LT} = \frac{G_f G_m}{G_m V_f + G_f V_m}
\]  

2-41

where

\[
\xi = \frac{(G_f / G_m) - 1}{(G_f / G_m) + \bar{\xi}}
\]  

2-43

and \( \bar{\xi} \) is reinforcing efficiency factor for in-plane shear.

Best agreement with experimental results has been found for \( \bar{\xi} = 1 \).

Figure 2-8 shows the variation of the shear modulus predicted by Eq. 2-42 with the fiber volume fraction. It may be pointed out that \( G_m \) (or \( E_m \)) has a significant influence on \( G_{LT} \) as \( E_m \) has on \( E_f \).
2.5. POISSON'S RATIO

When a unidirectional composite is loaded longitudinally, two Poisson ratios are defined, major Poisson ratio and minor Poisson ratio. *Major Poisson ratio* \((v_{LT})\) relates longitudinal stress to the transverse strain and *minor Poisson ratio* \((v_{TL})\) relates the transverse stress to the longitudinal strain.

The major Poisson ratio can be predicted using a constant stress model used for predicting transverse modulus, \(E_T\), by applying a load parallel to the fibers, that is,
parallel to the layers in the model. Figure 2-9 shows the deformation pattern for cumulative thickness of layers.

Figure 2-9 A unidirectional composite model for predicting Poisson’s ratio (adapted from [4])

Transverse deformations can be written as product of strain and cumulative thickness:

\[
\delta_f = t_f (\varepsilon_T)_f \\
\delta_m = t_m (\varepsilon_T)_m \\
\delta_c = t_c (\varepsilon_T)_c
\]

Substituting in Eq. 2-44 transverse strains in the fibers, matrix and composite as the product of longitudinal strains and Poisson ratios yields:

\[
\delta_f = -t_f v_f (\varepsilon_L)_f \\
\delta_m = -t_m v_m (\varepsilon_L)_m \\
\delta_c = -t_c v_c (\varepsilon_L)_c
\]
where $\nu_f$, $\nu_m$ and $\nu_c$ are the Poisson’s ratios of the fibers and matrix, respectively.

The deformation of the composite is the sum of the deformations of the fibers and the matrix. Therefore

$$\delta_c = \delta_f + \delta_m \quad 2-46$$

From Eq. 2-45 and 2-46

$$-t_c \nu_c (\varepsilon_L)_c = -t_f \nu_f (\varepsilon_L)_f - t_m \nu_m (\varepsilon_L)_m \quad 2-47$$

Since the longitudinal strains due to longitudinal stress in fiber, matrix and composite are equal, Eq. 2-47 becomes

$$t_c \nu_{LT} = t_f \nu_f + t_m \nu_m \quad 2-48$$

Dividing both sides of Eq. 2-48 by $t_c$ and substituting volume fraction for thickness yields

$$\nu_{LT} = \nu_f \nu_f + \nu_m \nu_m \quad 2-49$$

Eq. 2-49 represents Major Poisson ratio of a unidirectional composite.

Minor Poisson ratio is obtained from the following relation\(^2\):

$$\frac{\nu_{LT}}{\nu_{L}} = \frac{\nu_{TL}}{\nu_{T}} \quad 2-50$$

\(^2\) Derivation of Eq. 2-50 is given in chapter 3
2.6. SHORT-FIBER COMPOSITES

The properties of unidirectional composites discussed in previous sections have a special feature; the modulus in the direction of the fiber axis is higher than the one in transverse direction. Hence they are used in specific applications where the state of stress can be accurately determined. However, in applications where the state of stress is not predictable or approximately equal in all directions, unidirectional laminae may not be a good choice and thus a short-fiber composite is used. The composites containing short fibers as reinforcement are called short-fiber composites. They are also referred to as discontinuous-fiber reinforced composites. A short fiber composite with randomly oriented fibers in polymer matrix makes the overall composite behave as isotropic. Various aspects of this composite are discussed in this section.

2.6.1. MODULUS OF SHORT-FIBER COMPOSITES

The modulus of short fiber composites can be predicted using the stress distribution obtained through finite-element methods\(^3\) [9], [2] and [3]. The results are in the form of curves for specific properties of constituent materials. Whenever the properties change, a new set of results have to be obtained. Thus the results have limited adaptability to design procedures. For design purposes, it is usually desirable to have simple and rapid computational procedures for estimating composite properties even though the predictions are only approximate.

Halpin-Tsai [20] has developed simple and generalized semi-empirical equations to approximate the longitudinal and transverse moduli of aligned short-fiber composites (\(^\))

\(^3\) FEM approach to predict modulus of short fiber composites is beyond the scope of this thesis
Figure 2-10). The Halpin-Tsai equations for longitudinal and transverse moduli can be written as

\[
\frac{E_L}{E_m} = \frac{1 + (2l/d)\eta_L V_f}{1 - \eta_L V_f} \quad 2-51
\]

and

\[
\frac{E_T}{E_m} = \frac{1 + 2\eta_T V_f}{1 - \eta_T V_f} \quad 2-52
\]

where

\[
\eta_L = \frac{(E_f/E_m) - 1}{(E_f/E_m) + 2(l/d)} \quad 2-53
\]

and

\[
\eta_T = \frac{(E_f/E_m) - 1}{(E_f/E_m) + 2} \quad 2-54
\]

Figure 2-10 Model for aligned short-fiber composite
It may be noted here that Halpin-Tsai empirical relations for predicting transverse modulus of unidirectional composites and longitudinal and transverse modulus of short fiber composites are all particular cases of a general equation. The form of general equation coincides with that of transverse modulus for unidirectional composite 2-31, in which $\xi$ is a measure of reinforcement and is given by Eq. 2-33. The equations for longitudinal and transverse modulus of short fiber composites, Eq. 2-51 and 2-52, can be obtained from empirical relation presented for transverse modulus of unidirectional composites, Eq. 2-31, by substituting $(\xi = 2l/d)$ for the case of longitudinal modulus and $(\xi = 2)$ for the case of transverse modulus. The two values of $\xi$ are consistent with Eq. 2-33. Further, the Halpin-Tsai equations predict that the transverse modulus of an aligned short-fiber composite is not influenced by the fiber aspect ratio ($l/d$) and its value is same as that for the transverse modulus of a continuous-fiber composite. Figure 2-6 shows the predictions of Halpin-Tsai equation for transverse composite modulus as a function of fiber volume fraction for different constituent modulus ratios. Figure 2-11 and Figure 2-12 show the variations of the longitudinal modulus of aligned short fiber composites as functions of fiber aspect ratios for different fiber volume fractions and for modulus ratios 20 and 100.
Figure 2-11 Variation of longitudinal modulus of short-fiber composites against fiber aspect ratio for different volume fractions \( \frac{E_f}{E_m} = 20 \)
As mentioned earlier, randomly oriented short-fiber composites are produced to obtain composites that are essentially isotropic in a plane. The following empirical equations are often used to predict the elastic modulus and shear modulus of composites containing fibers that are randomly oriented in a plane:

\[
\begin{align*}
E_{\text{random}} & = \frac{3}{8} E_L + \frac{5}{8} E_T \\
G_{\text{random}} & = \frac{1}{8} E_L + \frac{1}{4} E_T
\end{align*}
\]
where $E_L$ and $E_T$ are respectively the longitudinal and transverse moduli of an aligned short-fiber composite having the same fiber aspect ratio and volume fraction as the composite under consideration. Moduli $E_L$ and $E_T$ can be determined using Eqs. 2-51 and 2-52.
CHAPTER 3. MECHANICS OF LAMINA AND LAMINATE

3.1. INTRODUCTION

One layer of a laminated composite material is generally referred to as a *ply* or *lamina*. It consists of single layer of reinforcement, unidirectional or multidirectional. It is too thin to be used for engineering applications. Several laminae are bonded together to form a structure called *laminate*. The properties and orientation of the laminae in a laminate are chosen to meet the laminate design requirements. The laminate properties can be predicted by knowing the properties of its constituents’ laminae. Also, the behavior of the laminate depends on the behavior of individual laminae. Hence for analysis or design of a laminate understanding the behavior of laminae is important. The analysis of laminae is discussed in section 3.2 and that of laminate in section 3.4. The methods presented in this chapter are already available in text books and papers. The reason of presenting them in this study is that they are fundamental for the developmental of methods presented in chapters 4 and 5.
3.2. MECHANICS OF LAMINA - HOOKE’S LAW FOR ORTHOTROPIC MATERIALS

From the mechanics standpoint, fiber composites are among the class of materials called orthotropic materials, whose behavior lies between that of isotropic and that of anisotropic materials.

Generally, the state of stress at a point is described by the nine components of the stress tensor, $\sigma_{ij}$, as shown in Figure 3-1. Correspondingly, there is a strain tensor, $\varepsilon_{ij}$, with nine components.

![Figure 3-1 Components of stress tensor (adapted from [4])](image)

The linear relationship that connects stress to strain is known as Hooke’s law and is expressed as:

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$$  \hspace{1cm} 3-1
where the components of fourth-order tensor $E_{ijkl}$ are known as elastic constants. As each stress component is related to all nine components of strain tensor, there are 81 elastic constants defining $E_{ijkl}$. Due to certain symmetry properties exhibited by this tensor, $E_{ijkl}$, the total number of independent components reduces to 21.

The first set of reductions in elastic constants is obtained by considering the symmetry of strain because of which, there is no loss of generality if $E_{ijkl}$ is assumed symmetric with respect to the last two indices.

$$E_{ijkl} = E_{ijlk}$$ \hspace{1cm} 3-2

This reduces the number of elastic constants from 81 to 54. By assuming $E_{ijkl}$ symmetric with respect to the first two indices because of the symmetry of the stress tensor reduces the number of constants further by 18 making the number of independent constants to 36.

$$E_{ijkl} = E_{jikl}$$ \hspace{1cm} 3-3

The final tally of 21 can be accomplished only by thermodynamic considerations. According to thermodynamics considerations, the strain energy density function can be assumed to exist as follows:

$$U = U(\varepsilon_{ij})$$ \hspace{1cm} 3-4

With the property

$$\frac{\partial U}{\partial \varepsilon_{ij}} = \sigma_{ij}$$ \hspace{1cm} 3-5
According to Eq. 3-1, $\sigma_{ij} = E_{ijkl} e_{kl}$, Therefore,

$$\frac{\partial U}{\partial e_{ij}} = E_{ijkl} e_{kl} \quad 3-6$$

Partial differentiation with respect to $e_{kl}$ yields,

$$\frac{\partial}{\partial e_{kl}} \left( \frac{\partial U}{\partial e_{ij}} \right) = E_{ijkl} \quad 3-7$$

Interchanging the indices in Eq. 3-7 gives,

$$\frac{\partial}{\partial e_{ij}} \left( \frac{\partial U}{\partial e_{kl}} \right) = E_{klij} \quad 3-8$$

Since the order of partial differentiation is immaterial,

$$\frac{\partial}{\partial e_{ij}} \left( \frac{\partial U}{\partial e_{kl}} \right) = \frac{\partial}{\partial e_{kl}} \left( \frac{\partial U}{\partial e_{ij}} \right) \quad 3-9$$

Hence by Eq. 3-9, it is evident that,

$$E_{ijkl} = E_{klij} \quad 3-10$$

Therefore, due to interchange of the first pair of indices with the second pair, the total number of independent elastic constants now reduces to 21 for a material that does not have any axes of symmetry. This type of material is called *aeolotropic* or *anisotropic*. Fiber composites come under the category of orthotropic materials that exhibit symmetry
of their elastic properties with respect to two orthogonal planes. Considering the axis of symmetry of orthotropic materials, the final $E_{ijkl}$ matrix is given as,

$$E_{ijkl} = \begin{bmatrix}
E_{1111} & E_{1122} & E_{1133} & 0 & 0 & 0 \\
E_{1122} & E_{2222} & E_{2233} & 0 & 0 & 0 \\
E_{1133} & E_{2233} & E_{3333} & 0 & 0 & 0 \\
0 & 0 & 0 & E_{2323} & 0 & 0 \\
0 & 0 & 0 & 0 & E_{1313} & 0 \\
0 & 0 & 0 & 0 & 0 & E_{1212}
\end{bmatrix} \quad 3-11$$

By careful observation of Eq. 3-11, it can be realized that four subscripts for the elastic tensor are not necessary to describe the nine nonzero elastic constants of orthotropic materials. Hence the Hooke’s law is modified as,

$$\sigma_i = Q_{ij} \varepsilon_j \quad i, j = 1,2,3,4,5,6 \quad 3-12$$

where $\sigma_i$ are the stress components, $Q_{ij}$ is the stiffness matrix and $\varepsilon_j$ are the engineering strain components. The engineering strains are different from the tensor strains used in Eq. 3-1. The two types of strains are described in [4]. The difference between the two arises only in the shearing strain components: $\gamma_{ij} = 2\varepsilon_{ij}$. An engineering shear strain is twice the corresponding tensorial shear strain. Eq. 3-12 can be written in matrix form as,
where the coordinate axes have been assumed to coincide with the symmetry axes of the material. Eq. 3-13 can be written for a two-dimensional case where all the terms related to the $x_3$ axis are dropped,

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \tau_{12} \end{pmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & 0 \\ Q_{12} & Q_{22} & 0 \\ 0 & 0 & Q_{66} \end{bmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \gamma_{12} \end{pmatrix}$$

It may be noted that whereas three-dimensional orthotropy requires nine independent elastic constants as shown in Eq. 3-13, only four constants are needed for two-dimensional orthotropy. For an isotropic material, the number of elastic constants required is only two for both two- and three-dimensional stress states. Due to the increased number of elastic constants there is additional complexity in orthotropic problems. The two-dimensional orthotropic problem is of primary concern in the remainder of this study.

### 3.3. STRESS-STRAIN RELATIONS AND ENGINEERING CONSTANTS

#### 3.3.1. SPECIALLY ORTHOTROPIC LAMINA

Consider an orthotropic lamina shown in Figure 3-2, with the reference axes coinciding with the axes of symmetry and designated as the longitudinal direction, L, and the transverse direction, T. The engineering constants that define the material property of this lamina are the longitudinal modulus ($E_L$), transverse modulus ($E_T$), shear modulus ($G_{LT}$), major Poisson’s ratio ($\nu_{LT}$) and minor Poisson’s ratio ($\nu_{TL}$).
Figure 3-2 Specially orthotropic lamina (adapted from [4])

The significance of these constants can be explained by considering the deformation response of the lamina as shown in Figure 3-3, to the following states of stress:

i. When $\sigma_L$ is the only nonzero stress ($\sigma_T = \tau_{LT} = 0$), the strains produced are

$$\varepsilon_L = \frac{\sigma_L}{E_L}$$  \hspace{1cm} 3-15

$$\varepsilon_T = -v_{LT} \varepsilon_L = -v_{LT} \frac{\sigma_L}{E_L}$$  \hspace{1cm} 3-16

$$\gamma_{LT} = 0$$  \hspace{1cm} 3-17

ii. When $\sigma_T$ is the only nonzero stress ($\sigma_L = \tau_{LT} = 0$), the strains produced are

$$\varepsilon_T = \frac{\sigma_T}{E_T}$$  \hspace{1cm} 3-18

$$\varepsilon_L = -v_{TL} \varepsilon_T = -v_{TL} \frac{\sigma_T}{E_T}$$  \hspace{1cm} 3-19
\( \gamma_{LT} = 0 \)  \hspace{1cm}  \text{(3-20)}

iii. When \( \tau_{LT} \) is the only nonzero stress (\( \sigma_L = \sigma_T = 0 \)), the strains produced are

\[ \varepsilon_L = 0 \]  \hspace{1cm}  \text{(3-21)}

\[ \varepsilon_T = 0 \]  \hspace{1cm}  \text{(3-22)}

\[ \gamma_{LT} = \frac{\tau_{LT}}{G_{LT}} \]  \hspace{1cm}  \text{(3-23)}

Considering the assumption of linearly elastic material, the strains produced by the three stresses, as given by Eq. 3-15 to Eq. 3-23 can be superposed to give the following relations:

\[ \varepsilon_L = \frac{\sigma_L}{E_L} - v_{LT} \frac{\sigma_T}{E_T} \]  \hspace{1cm}  \text{(3-24)}

\[ \varepsilon_T = \frac{\sigma_T}{E_T} - v_{LT} \frac{\sigma_L}{E_L} \]  \hspace{1cm}  \text{(3-25)}

\[ \gamma_{LT} = \frac{\tau_{LT}}{G_{LT}} \]  \hspace{1cm}  \text{(3-26)}
Figure 3-3 Deformation response of an orthotropic lamina. Undeformed lamina shown in broken lines. (adapted from [4])
3.3.2. RELATIONS BETWEEN ENGINEERING CONSTANTS AND ELEMENTS OF STIFFNESS AND COMPLIANCE MATRICES

In this section the relation between the five engineering constants of Eqs. 3-24 - 3-26 and four independent elastic constants of Eq. 3-14 is derived by subjecting the lamina to the stress states considered in section 3.3.1 and comparing the strains obtained in section 3.3.1 with those obtained using Eq. 3-14. First consider that \( \sigma_L \) is the only nonzero stress. With the substitution of \( \sigma_L = \tau_{LT} = 0 \), Eq. 3-14 can be written as

\[
\sigma_L = Q_{11} \epsilon_L + Q_{12} \epsilon_T
\]

\[
\sigma_T = 0 = Q_{12} \epsilon_L + Q_{22} \epsilon_T
\]

Solving for \( \epsilon_L \) and \( \epsilon_T \) gives,

\[
\epsilon_L = \frac{Q_{22}}{Q_{11}Q_{22} - Q_{12}^2} \sigma_L
\]

\[
\epsilon_T = \frac{Q_{12}}{Q_{11}Q_{22} - Q_{12}^2} \sigma_L
\]

Comparing Eqs. 3-27 and 3-28 with 3-15 and 3-16

\[
E_L \equiv \frac{\sigma_L}{\epsilon_L} = \frac{Q_{11}Q_{22} - Q_{12}^2}{Q_{22}}
\]

and

\[
v_{LT} \equiv -\frac{\epsilon_T}{\epsilon_L} = \frac{Q_{12}}{Q_{22}}
\]
Repeating the above operation with $\sigma_r$ as the only nonzero stress in Eq. 3-14 yields

$$E_T \equiv \frac{\sigma_r}{\varepsilon_r} = \frac{Q_{11}Q_{22} - Q_{12}^2}{Q_{11}}$$ \hspace{1cm} 3-31

and

$$v_{LT} \equiv \frac{\varepsilon_L}{\varepsilon_T} = \frac{Q_{12}}{Q_{11}}$$ \hspace{1cm} 3-32

Finally, if $\tau_{LT}$ is the only nonzero stress,

$$G_{LT} \equiv \frac{\tau_{LT}}{\gamma_{LT}} = Q_{66}$$ \hspace{1cm} 3-33

Solving Eqs. 3-29 to 3-32 for three components of stiffness matrix and writing the fourth component from Eq. 3-33 will yield,

$$Q_{11} = \frac{E_L}{1 - v_{LT}v_{TL}}$$

$$Q_{22} = \frac{E_T}{1 - v_{LT}v_{TL}}$$ \hspace{1cm} 3-34

$$Q_{12} = \frac{v_{LT}E_T}{1 - v_{LT}v_{TL}} = \frac{v_{TL}E_L}{1 - v_{LT}v_{TL}}$$

$$Q_{66} = G_{LT}$$

From Eq. 3-34 it is evident that only four of the five engineering constants are independent. The following functional relationship exists between four of the five constants:

$$v_{LT}E_T = v_{TL}E_L$$ \hspace{1cm} 3-35
3.3.3. STRESS STRAIN RELATIONS FOR GENERALLY ORTHOTROPIC LAMINA

A lamina is typically stacked with several other unidirectional laminae in a specified sequence of orientation to form a laminate. Thus, the principal material directions of each lamina make a different angle, $\theta$, with a common set of reference axes. The stress-strain relationships of each lamina with respect to its principal material directions are given in the previous section. This section highlights the stress-strain relationships of a lamina to a common-reference coordinate system. A lamina referred to arbitrary axes is called a *generally orthotropic lamina*.

Consider a lamina as shown in Figure 3-4. The principal material axes are oriented at an angle $\theta$ with the reference coordinate axes. Stresses and strains can be easily transformed from one set of axes to other using the following transformation relations:

$$
\begin{bmatrix}
\sigma_L \\
\sigma_T \\
\tau_{LT}
\end{bmatrix} =
\begin{bmatrix}
\sigma_s \\
\sigma_y \\
\tau_{xy}
\end{bmatrix}
\begin{bmatrix}
T_1 \\
T_2 \\
T_3
\end{bmatrix}
$$

or

$$
\frac{V_{LT}}{E_L} = \frac{V_{TL}}{E_T}
$$

and

$$
3-36
$$
\[
\begin{bmatrix}
\varepsilon_L \\
\varepsilon_T \\
\frac{1}{2}\gamma_{LT} \\
\frac{1}{2}\gamma_{xy}
\end{bmatrix} = [T]\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\end{bmatrix}
\]

3-37

where transformation matrix \([T]\) is given by

\[
[T] = \begin{bmatrix}
\cos^2 \theta & \sin^2 \theta & 2(\sin \theta)(\cos \theta) \\
\sin^2 \theta & \cos^2 \theta & -2(\sin \theta)(\cos \theta) \\
-(\sin \theta)(\cos \theta) & (\sin \theta)(\cos \theta) & \cos^2 \theta - \sin^2 \theta
\end{bmatrix}
\]

3-38

In Eq. 3-38, the angle \(\theta\) is to be taken positive when the angle of L-T axes measured from x-y axes is in the counterclockwise direction. In Eq. 3-37, tensor strains are to be used and not engineering strains. The inverted form of Eq. 3-36 is obtained by pre-multiplying both sides of the equation by \([T]^{-1}\):

\[
\begin{bmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{bmatrix} = [T]^{-1}\begin{bmatrix}
\sigma_L \\
\sigma_T \\
\tau_{LT}
\end{bmatrix}
\]

3-39

where the inverse of the transformation matrix is obtained by replacing \(\theta\) by \(-\theta\)

\[
[T]^{-1} = \begin{bmatrix}
\cos^2 \theta & \sin^2 \theta & -2(\sin \theta)(\cos \theta) \\
\sin^2 \theta & \cos^2 \theta & 2(\sin \theta)(\cos \theta) \\
-(\sin \theta)(\cos \theta) & (\sin \theta)(\cos \theta) & \cos^2 \theta - \sin^2 \theta
\end{bmatrix}
\]

3-40

The stress-strain relations in principal material directions are given in matrix form in Eq. 3-14. Replacing the engineering strains by tensorial strains yield,
Substituting Eq. 3-37 into Eq. 3-41 yields,

\[
\begin{bmatrix}
\sigma_L \\
\sigma_T \\
\tau_{LT}
\end{bmatrix} =
\begin{bmatrix}
Q_{11} & Q_{12} & 0 \\
Q_{12} & Q_{22} & 0 \\
0 & 0 & 2Q_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_L \\
\varepsilon_T \\
\frac{1}{2}\gamma_{LT}
\end{bmatrix}
\]  
3-41

Substituting Eq. 3-42 into Eq. 3-39 yields,

\[
\begin{bmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{bmatrix} = [T]^{-1}
\begin{bmatrix}
Q_{11} & Q_{12} & 0 \\
Q_{12} & Q_{22} & 0 \\
0 & 0 & 2Q_{66}
\end{bmatrix}
[T]
\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\frac{1}{2}\gamma_{xy}
\end{bmatrix}
\]  
3-42

Substituting Eq. 3-42 into Eq. 3-39 yields,

\[
\begin{bmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{bmatrix} = [T]^{-1}
\begin{bmatrix}
Q_{11} & Q_{12} & 0 \\
Q_{12} & Q_{22} & 0 \\
0 & 0 & 2Q_{66}
\end{bmatrix}
[T]
\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\frac{1}{2}\gamma_{xy}
\end{bmatrix}
\]  
3-43

Eq. 3-43 gives the stress-strain equation for an orthotropic lamina referred to arbitrary axes. For uniformity, a \([\overline{Q}]\) matrix similar to \([Q]\) matrix of Eq. 3-14 is defined that relates engineering strains to the stresses referred to arbitrary axes. Thus,

\[
\begin{bmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{bmatrix} =
\begin{bmatrix}
\overline{Q}_{11} & \overline{Q}_{12} & \overline{Q}_{16} \\
\overline{Q}_{12} & \overline{Q}_{22} & \overline{Q}_{26} \\
\overline{Q}_{16} & \overline{Q}_{26} & \overline{Q}_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\gamma_{xy}
\end{bmatrix}
\]  
3-44

where,

\[
\begin{align*}
\overline{Q}_{11} &= Q_{11}\cos^4\theta + Q_{22}\sin^4\theta + 2(Q_{12} + 2Q_{66})\sin^2\theta \cdot \cos^2\theta \\
\overline{Q}_{22} &= Q_{11}\sin^4\theta + Q_{22}\cos^4\theta + 2(Q_{12} + 2Q_{66})\sin^2\theta \cdot \cos^2\theta \\
\overline{Q}_{12} &= (Q_{11} + Q_{22} - 4Q_{66})\sin^2\theta \cdot \cos^2\theta + Q_{12}(\cos^4\theta + \sin^4\theta) \\
\overline{Q}_{66} &= (Q_{11} + Q_{22} - 2Q_{12} - 2Q_{66})\sin^2\theta \cdot \cos^2\theta + Q_{12}(\cos^4\theta + \sin^4\theta) \\
\overline{Q}_{16} &= (Q_{11} - Q_{12} - 2Q_{66})\sin\theta \cdot \cos^3\theta - (Q_{22} - Q_{12} - 2Q_{66})\cos\theta \cdot \sin^3\theta \\
\overline{Q}_{26} &= (Q_{11} - Q_{12} - 2Q_{66})\sin^3\theta \cdot \cos\theta - (Q_{22} - Q_{12} - 2Q_{66})\cos^3\theta \cdot \sin\theta
\end{align*}
\]  
3-45
3.4. MECHANICS OF LAMINATE

A laminate is a stacked structural element of two or more laminae. The laminae are bonded together with principal material directions oriented in a way to produce a structural element with the desired properties in all directions. In subsequent sections, the analysis of laminates is discussed from the known properties of the constituent laminae.

3.5. STRAIN AND STRESS VARIATION IN A LAMINATE

Several laminae are bonded together in such a way that a laminate act as a single-layer material. The bond between adjacent laminae is assumed to be perfect, that is, infinitesimally thin and not shear deformable. Thus the laminae cannot slip over each other, and the displacements remain continuous across the bond. In this section equations are developed that relate the strain at any point in a laminate to the displacements and curvatures of its geometric midplane. But since the laminate is made of several laminae
with different directional properties, the variation of the stress across the thickness of the laminate is discussed.

Consider the deformation of a section of a laminate in the $x$-$z$ plane as shown in Figure 3-5. Assume that the laminae over the cross section do not slip and neglect shear deformations $\gamma_{xz}$ and $\gamma_{yz}$. These assumptions are equivalent to the assumption that the line $ABCD$ which is straight and perpendicular to the midplane of the laminate in the undeformed state remains straight and perpendicular to the midplane after deformation. Further assume that the point $B$ at the geometric midplane undergoes displacements $u_0$, $v_0$, and $w_0$ along $x$, $y$, and $z$ directions respectively.

![Figure 3-5 Bending of line element in x-z plane (adapted from [4])](image)

The displacement of point $C$ located at a distance $z$ on the normal $ABCD$ from the midplane is given by,

$$u = u_0 - z\alpha$$

3-46
where $\alpha$ is the slope of the laminate midplane in the $x$ direction. Substituting $\alpha = \frac{\partial w_0}{\partial x}$ in Eq. 3-46 will yield

$$u = u_0 - z \frac{\partial w_0}{\partial x}$$  \hspace{1cm} 3-47

Similarly, the displacement, $v$, in the $y$ direction is,

$$v = v_0 - z \frac{\partial w_0}{\partial y}$$  \hspace{1cm} 3-48

and the displacement, $w$, in the $z$ direction is,

$$w = w_0$$  \hspace{1cm} 3-49

In Eq. 3-49 the stretching (or shortening) of the normal is neglected since it is insignificant when compared to the displacement $w_0$. Therefore, the normal strains, $\varepsilon_z$, are neglected which reduces the laminate strains to $\varepsilon_x$, $\varepsilon_y$ and $\gamma_{xy}$. These strains for the derived displacements are as follows:

$$\varepsilon_x = \frac{\partial u}{\partial x} = \frac{\partial u_0}{\partial x} - z \frac{\partial^2 w_0}{\partial x^2}$$

$$\varepsilon_y = \frac{\partial v}{\partial y} = \frac{\partial v_0}{\partial y} - z \frac{\partial^2 w_0}{\partial y^2}$$  \hspace{1cm} 3-50

$$\gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = \frac{\partial u_0}{\partial y} + \frac{\partial v_0}{\partial x} - 2z \frac{\partial^2 w_0}{\partial x \partial y}$$

The strain-displacements relationships of Eq. 3-50 in terms of the midplane strains and the plate curvatures are as follows:

$$\begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{bmatrix} = \begin{bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{bmatrix} + z \begin{bmatrix} \kappa_x \\ \kappa_y \\ \kappa_{xy} \end{bmatrix}$$  \hspace{1cm} 3-51
where the midplane strains are

\[
\begin{pmatrix}
\varepsilon_x^0 \\
\varepsilon_y^0 \\
\gamma_{xy}^0
\end{pmatrix} = \begin{pmatrix}
\frac{\partial u_0}{\partial x} \\
\frac{\partial v_0}{\partial y} + \frac{\partial u_0}{\partial x} \\
\frac{\partial u_0}{\partial y} + \frac{\partial v_0}{\partial x}
\end{pmatrix}
\]  \hspace{1cm} \text{(3-52)}

and the plate curvatures are

\[
\begin{pmatrix}
\kappa_x \\
\kappa_y \\
\kappa_{xy}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial^2 w_0}{\partial x^2} \\
\frac{\partial^2 w_0}{\partial y^2} \\
2 \frac{\partial^2 w_0}{\partial x \partial y}
\end{pmatrix}
\]  \hspace{1cm} \text{(3-53)}

Eq. 3-51 indicates that the strains in a laminate vary linearly across its thickness. Stresses in any lamina (e.g., \( r^{th} \)) can be obtained by substituting Eq. 3-51 in the stress-strain relation, Eq. 3-44,

\[
\begin{pmatrix}
\sigma_x \\
\sigma_y \\
\tau_{xy}
\end{pmatrix}_r = \begin{bmatrix}
\overline{Q}_{11} & \overline{Q}_{12} & \overline{Q}_{16} \\
\overline{Q}_{12} & \overline{Q}_{22} & \overline{Q}_{26} \\
\overline{Q}_{16} & \overline{Q}_{26} & \overline{Q}_{66}
\end{bmatrix}_r \begin{pmatrix}
\varepsilon_x^0 \\
\varepsilon_y^0 \\
\gamma_{xy}^0
\end{pmatrix} + \begin{pmatrix}
\overline{Q}_{11} & \overline{Q}_{12} & \overline{Q}_{16} \\
\overline{Q}_{12} & \overline{Q}_{22} & \overline{Q}_{26} \\
\overline{Q}_{16} & \overline{Q}_{26} & \overline{Q}_{66}
\end{pmatrix}_r \begin{pmatrix}
\kappa_x \\
\kappa_y \\
\kappa_{xy}
\end{pmatrix}_r
\]  \hspace{1cm} \text{(3-54)}

Thus the stress variation through the laminate thickness is obtained by calculating the stress variations in all the laminae.

### 3.6. SYNTHESIS OF STIFFNESS MATRIX

Since the stresses in a laminate vary from layer to layer, it is convenient to deal with a simpler but equivalent system of forces and moments acting on a laminate cross section. Thus the resultant forces and moments are obtained by integrating the
corresponding stress through a laminate thickness, $h$, and integrating the corresponding stress times the moment arm with respect to the midplane respectively:

$$N_x, M_x = \int_{-h/2}^{h/2} \sigma_x(1, z)dz$$

$$N_y, M_y = \int_{-h/2}^{h/2} \sigma_y(1, z)dz$$

$$N_{xy}, M_{xy} = \int_{-h/2}^{h/2} \tau_{xy}(1, z)dz$$

where $N_x, N_y$, and $N_{xy}$ have units of force per unit length (e.g., width of the beam) and $M_x, M_y$, and $M_{xy}$ have units of moment per unit length.

It is convenient to replace the continuous integrals by summation of integrals to find the force-moment system. To keep track of integrations, each ply should be numbered. The convention for numbering of plies and finding distances of each ply from the mid-plane is shown in Figure 3-6:

$$\begin{align*}
N_x &= \int_{-h/2}^{h/2} \sigma_x \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \sigma_x \frac{dz}{h}
N_y &= \int_{-h/2}^{h/2} \sigma_y \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \sigma_y \frac{dz}{h}
N_{xy} &= \int_{-h/2}^{h/2} \tau_{xy} \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \tau_{xy} \frac{dz}{h}
\end{align*}$$

and

$$\begin{align*}
N_x &= \int_{-h/2}^{h/2} \sigma_x \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \sigma_x \frac{dz}{h}
N_y &= \int_{-h/2}^{h/2} \sigma_y \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \sigma_y \frac{dz}{h}
N_{xy} &= \int_{-h/2}^{h/2} \tau_{xy} \left( \frac{z}{h} \right) \frac{dz}{h} = \sum_{k=1}^{n} \int_{z_{k-1}}^{z_k} \tau_{xy} \frac{dz}{h}
\end{align*}$$
Substituting stresses from Eq. 3-54 and simplifying will yield,

\[
\begin{align*}
\begin{bmatrix} N_x \\ N_y \\ N_{xy} \end{bmatrix} &= \begin{bmatrix} A_{11} & A_{12} & A_{16} \\ A_{12} & A_{22} & A_{26} \\ A_{16} & A_{26} & A_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{bmatrix} + \begin{bmatrix} B_{11} & B_{12} & B_{16} \\ B_{12} & B_{22} & B_{26} \\ B_{16} & B_{26} & B_{66} \end{bmatrix} \begin{bmatrix} \kappa_x \\ \kappa_y \\ \kappa_{xy} \end{bmatrix} \\
M_x &= \begin{bmatrix} B_{11} & B_{12} & B_{16} \\ B_{12} & B_{22} & B_{26} \\ B_{16} & B_{26} & B_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{bmatrix} + \begin{bmatrix} D_{11} & D_{12} & D_{16} \\ D_{12} & D_{22} & D_{26} \\ D_{16} & D_{26} & D_{66} \end{bmatrix} \begin{bmatrix} \kappa_x \\ \kappa_y \\ \kappa_{xy} \end{bmatrix} \\
M_{xy} &= \begin{bmatrix} B_{11} & B_{12} & B_{16} \\ B_{12} & B_{22} & B_{26} \\ B_{16} & B_{26} & B_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{bmatrix} + \begin{bmatrix} D_{11} & D_{12} & D_{16} \\ D_{12} & D_{22} & D_{26} \\ D_{16} & D_{26} & D_{66} \end{bmatrix} \begin{bmatrix} \kappa_x \\ \kappa_y \\ \kappa_{xy} \end{bmatrix}
\end{align*}
\]

where,

\[
A_{ij} = \sum_{k=1}^{n} \left( \overline{O}_{ij} \right)_k (h_k - h_{k-1})
\]

\[
B_{ij} = (1/2) \sum_{k=1}^{n} \left( \overline{O}_{ij} \right)_k (h_k^2 - h_{k-1}^2)
\]

\[
D_{ij} = (1/3) \sum_{k=1}^{n} \left( \overline{O}_{ij} \right)_k (h_k^3 - h_{k-1}^3)
\]

Combining Eq. 3-58, 3-59 and 3-60, the total plate constitutive equation is written as:
Eq. 3-61 in concise form is,
\[
\begin{bmatrix}
N_x \\
N_y \\
N_{xy}
\end{bmatrix} = 
\begin{bmatrix}
A_{11} & A_{12} & A_{16} & B_{11} & B_{12} & B_{16} \\
A_{12} & A_{22} & A_{26} & B_{12} & B_{22} & B_{26} \\
A_{16} & A_{26} & A_{66} & B_{16} & B_{26} & B_{66}
\end{bmatrix}
\begin{bmatrix}
\epsilon_x^0 \\
\epsilon_y^0 \\
\gamma_{xy}^0
\end{bmatrix}
\]  \hspace{1cm} 3-61

In Eq. 3-62 the matrices \( A, B, \) and \( D \) are called the *extensional stiffness matrix*, *coupling stiffness matrix*, and *bending stiffness matrix* respectively. The external stiffness matrix relates the resultant forces to the midplane strains, and the bending stiffness matrix relates the resultant moments to the plate curvatures. Together \( A, B, \) and \( D \) form stiffness matrix \( C \) which will be used as input for the failure and the reliability model developed by Hammitt [21].
\[
\begin{bmatrix}
N \\
M
\end{bmatrix} = 
\begin{bmatrix}
A & B \\
B & D
\end{bmatrix}
\begin{bmatrix}
\epsilon^0 \\
\kappa
\end{bmatrix}
\]  \hspace{1cm} 3-62

The flowchart for the relation between the conventional composite model (models presented in chapters 2 and 3 that predict the stiffness matrix of a conventional composite Eq. 3-63) and the failure and reliability analysis model developed by Hammitt [21] is shown in Figure 3-7. The input for the conventional composite model consists of the properties of fiber and matrix along with the respective volume fractions and the output of conventional composite model is the stiffness matrix of the composite. This will act as
input for the failure and reliability model [21]. The output of the failure and reliability models is the load deflection history of conventional composite plate.

![Flowchart](image)

**Figure 3-7 Flow of information between various models and methods for deterministic analysis of plates made of conventional and nanocomposites**

### 3.7. NUMERICAL EXAMPLES

The computed stiffness matrix of a conventional composite material, Eq. 3-63, will be used as input to the failure analysis model developed by Hammitt [21]. The example problem presented here has been also presented in Pilla et al.[35].

The post buckling response of a flat rectangular graphite-epoxy plate was analyzed. Figure 4-7 shows the properties and geometry of the plate (Source: Hammitt [21]). The finite element mesh consisted of 12 elements in the $x$ direction and 6 elements along the $y$
direction. The load, $P$, was distributed across the edge of the plate. The total applied load is 2100 N.

Out-of-plane displacement at the point of maximum nodal deflection was computed and is plotted against load as shown in Figure 3-9. The load is normalized by $P_{cr}$, which is the critical load at which buckling would occur for a perfect plate. The postbuckling strengthening is due to the constraint of the deflection, $w$, of the side and loading edges of the plate. The results found to be in good agreement with experimental and published results by Starnes [44] and Elseifi [15] respectively.

**Figure 3-8 Properties and geometry of Graphite Epoxy Plate (Source: Hammit [21])**

<table>
<thead>
<tr>
<th>Conventional Composite Lamina Properties:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_L = 131.0$ GPa</td>
</tr>
<tr>
<td>$E_T = 13.0$ GPa</td>
</tr>
<tr>
<td>$G_{LT} = 6.4$ GPa</td>
</tr>
<tr>
<td>$v_{LT} = 0.38$</td>
</tr>
<tr>
<td>$t_i = 0.14$ mm</td>
</tr>
<tr>
<td>Stacking Sequence:</td>
</tr>
<tr>
<td>$[\pm 45/0_2, \pm 45/0_2, \pm 43/0/90]_6$</td>
</tr>
<tr>
<td>(24 plies)</td>
</tr>
</tbody>
</table>

**Figure 3-9 Load-deflection Curve for a Conventional Composite Plate with Postbuckling Strength**
4.1. INTRODUCTION

To increase the understanding of the mechanical behavior of nanofiber/nanotube reinforced polymers, there is a need to develop theory that can predict the effective properties of these materials. The theory can be determined by a select set of computational methods. These modeling methods span a wide range of length and time scales, as shown in Figure 4-1. For the extremities, i.e. the smallest and largest length and time scales, Computational Chemistry techniques and Computational Mechanics, based on thoroughly established principles developed in science and engineering, are used to predict atomic structure (using first principles) and mechanical behavior of materials and engineering structures respectively. However, the intermediate length and time scales do not have general modeling methods that are as well-developed as those on the smallest and largest time and length scales. Therefore, multiscale modeling techniques are employed, which take advantage of Computational Chemistry and Computational Mechanics methods simultaneously for the prediction of the structure and properties of materials [48].
As shown in Figure 4-1, each modeling method is associated with relevant modeling tools. The Quantum mechanical and nanomechanical modeling tools assume the presence of a discrete molecular structure of matter. Micromechanical and Structural Mechanics assume the presence of a continuous material structure.

Figure 4-2 shows the relationship of specific modeling techniques in Computational Mechanics and Computational Chemistry. The continuum-based methods are classified as micromechanics and structural mechanics. The former is further sub-divided into analytical micromechanics which include Mori-Tanaka, Eshelby approach, Halpin-Tsai approach and computational micromechanics which include Finite Element Method (FEM), the Boundary Element Method (BEM) [1], [7], [10], [16], [22]-[26], [33]. The molecular modeling tools include molecular dynamics, Monte Carlo, and Ab-initio techniques.

Figure 4-1 various length and time scales used in determining mechanical properties of nanocomposites (adapted from [48])
Since this study assumes the material to be continuum, the modeling technique to be used should be of continuous molecular structure i.e. length scale of $10^{-6}$. Therefore a micromechanics method is used. Since the objective is to develop a theory, computational micromechanics cannot be used. Therefore, the author used traditional micromechanics method such as Mori-Tanaka to predict the behavior of nanocomposites.

4.2. MORI-TANAKA METHOD

The Mori-Tanaka micromechanical method has been used by many researchers [18], [42] to model the effective behavior of nanocomposites. It allows the average stress fields and overall effective stiffness of a composite with a non-dilute concentration of
inclusions to be determined. It has been extended by Benveniste [8] and Weng [50] to cover composites with multiple inclusion phases and by Tandon et al. [45] and Weng [50] to cover random orientations of inclusions.

In the current study, Mori-Tanaka solution for a two phase composite is of interest. One phase is inclusion (nanofiber/nanotube, assumed to be straight) and the other is polymer matrix. First the case where the inclusions are unidirectionally aligned within the matrix is considered. Once the necessary parameters have been determined for this case, appropriate averaging techniques are applied to arrive at the solution for randomly oriented inclusions. Presented briefly in subsequent sections is stiffness matrix of nanocomposite (aligned and randomly oriented inclusions). For detailed derivation, the reader is directed to [17].

4.2.1. MORI-TANAKA METHOD FOR ALIGNED INCLUSIONS

Consider a composite with aligned inclusions. The Mori-Tanaka [33] method assumes that each inclusion is embedded in a matrix subjected to an effective stress \( \sigma_m \) or an effective strain \( \varepsilon_m \) in the far field, where \( \sigma_m \) and \( \varepsilon_m \) denote the average stress and the average strain over the matrix respectively. The stiffness tensor \( C \) of the composite reinforced by aligned inclusions is given by:

\[
C = (V_mC_m + V_rC_r : A) : (V_mI + V_rA)^{-1}
\]

\[4-1\]

\( I \) is the fourth order identity tensor. \( A \) is the fourth order dilute strain concentration tensor that relates average strains \( \varepsilon_r \) and \( \varepsilon_m \),
\[ \varepsilon_r = A : \varepsilon_m \]  
\[ A = \left[ I + S : (C_m)^{-1} : (C_r - C_m) \right]^{-1} \]

\( S \) is the standard Eshelby tensor [16], [18], [42]; colon between two tensors denotes contraction (inner product) over two indices; subscripts \( m \) and \( r \) indicate the matrix and reinforcing phase, respectively, \( V_m \) and \( V_r \) denote the volume fractions, and \( C_m \) and \( C_r \) denote the tensors of the elastic moduli of the corresponding phases.

### 4.2.2. MORI-TANAKA METHOD FOR RANDOMLY ORIENTED INCLUSIONS

In this section we consider composites with randomly oriented inclusions. The term “randomly oriented inclusion” means an inclusion has same probability to be oriented in any direction. The stiffness tensor \( C \) of the composite reinforced by randomly oriented inclusions is given by:

\[ C = \left( V_mC_m + V_r \{ C_r : A \} \right) : \left( V_mI + V_r \{ A \} \right)^{-1} \]

The curly brackets \( \{ \} \) represent orientational average [42] (average over all possible orientations of the inclusion).

### 4.2.3. EULER ANGLES AND TENSOR TRANSFORMATIONS

As seen in Eq. 4-4, the orientational averages of tensors have to be calculated in order to determine the effective properties of a nanocomposite with randomly oriented inclusions. This section highlights the tensor transformations and Euler angles necessary for orientational average. For detailed analysis refer [17].
Assume the local axis of the inclusion is denoted by $x_1^i$, $x_2^i$ and $x_3^i$ and the global axis by $X_1^i$, $X_2^i$ and $X_3^i$ (Figure 4-3). Also assume the inclusion is oriented in 3-direction.

![Figure 4-3 Relationship between the local and global coordinate system (adapted from [42])](image)

The objective is to develop the transformation matrix $a_{ij}$ which maps vector $v_j^i$ in the local coordinate system to coordinates $v^i$ in the global coordinate system.

$$v^i = a_{ij} v_j^i$$ \hspace{1cm} 4-5

In general it is necessary to specify three Euler angles to describe inclusion orientation but here since the inclusion is assumed to be spheroidal it is enough to specify $\Phi_1$ and $\Phi$ in Figure 4-3.

Following the transformations (rotation of axes with respect to the angles specified), the local and global vectors are related by Eq.4-6,
\[
\begin{bmatrix}
X_1 \\
X_2 \\
X_3
\end{bmatrix} = \begin{bmatrix}
ab & -c & ad \\
bc & a & cd \\
-d & 0 & b
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
\]

\[4-6\]

\[a = \cos\phi_1, \ b = \cos\Phi, \ a = \sin\phi_1, \ d = \sin\Phi\]

Eq. 4-6 can also be written as,

\[X_i = A_{ij}x_j\]

\[4-7\]

Where \(A_{ij}\) represents the transformation matrix for a three-dimensional space.

For higher order tensor transformations, the usual tensor transformation laws are accomplished. Thus the transformation of a fourth order stiffness tensor \(C_{ijkl}\) from local to global coordinates can be written as,

\[C_{ijkl}(\phi_1, \Phi) = A_{ip}A_{jk}A_{kl}A_{lu}C'_{mun}\]

\[4-8\]

Given Eq. 4-8, the orientational average of a fourth order tensor in 3D space is,

\[\{C_{ijkl}\} = \frac{1}{2\pi} \int_0^{2\pi} \int_0^\pi C_{ijkl}(\phi_1, \Phi)\sin(\Phi)d\Phi d\phi_1\]

\[4-9\]

where the transformation matrix for three-dimensional space from Eq. 4-7 is used in Eq. 4-8 and the \(\sin(\Phi)\) term accounts for the surface area of a sphere.

For a 3D random orientation of inclusions, the stiffness tensor transformations in contracted notation can be written in matrix form as:
Figure 4-4 and Figure 4-5 show the variation of composite modulus with volume fraction of inclusions for unidirectional and random cases respectively. These results obtained by Eq. 4-1 and Eq. 4-4 suggest that small amounts of carbon nanotubes/nanofibers can significantly enhance the overall mechanical behavior of the polymer. This observation has been validated experimentally [6], [19], [37], [39], [40].
Figure 4-4 Effect of Volume Fraction on Elastic Modulus of a Nanocomposite Material with Unidirectional Straight Inclusions
The flowchart for the relation between micromechanical model that predicts the stiffness matrix of nanocomposite and failure and reliability analysis model developed by Hammitt [21] is shown in Figure 4-6. The input for the micromechanical model is properties of nanofiber/nanotube and polymer matrix along with respective volume fractions and the output of micromechanical model is the stiffness matrix. This will act as input for the failure and reliability model [21]. The output of failure and reliability model is load deflection history of nanocomposite plate.
4.3. NUMERICAL EXAMPLES

The computed stiffness matrix of nanocomposite, Eq. 4-1 or Eq. 4-4, will be used as input for failure analysis model developed by Hammitt [21]. The same example problem presented in Pilla et al.[35] will be solved for load-deflection history.

The post buckling response of a flat rectangular graphite-epoxy plate was analyzed. Figure 4-7 gives the properties and geometry (Source: Hammitt [21]) of the plate. The finite element mesh consisted of 12 elements in the x direction and 6 elements along the y direction. The load was distributed across the edge of the plate. The nanofibers/nanotubes are randomly oriented in the polymer matrix. The total applied load is 2100 N.

Figure 4-8 shows the postbuckling response for plates with volume fractions of nanofiber/nanotube of 5% and 10%. As expected, the plate with a higher volume fraction
of the nanofiber/nanotube exhibits greater strength than the plate with lower volume fraction.

<table>
<thead>
<tr>
<th>Nano Composite</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_f = 200000$ MPa</td>
</tr>
<tr>
<td>$E_w = 1900$ MPa</td>
</tr>
<tr>
<td>$\nu_f = 0.3$</td>
</tr>
<tr>
<td>$\nu_w = 0.3$</td>
</tr>
<tr>
<td>$V_f = 5% - 10%$</td>
</tr>
</tbody>
</table>

Figure 4-7 Properties and geometry of Graphite Epoxy Plate (Source: Hammitt [21])

Figure 4-8 Load-deflection Curve for a Nanocomposite Plate with Postbuckling Strength
CHAPTER 5. AN ENCAPSULATED INCLUSION MODEL FOR INTERFACE MODELING OF CARBON NANOTUBE/NANOFIBER COMPOSITES

5.1. INTRODUCTION

A continuum-based micromechanical model is developed that takes into consideration the interface between CNT/CNF and matrix to compute the overall nanocomposite elastic modulus. The model assumes that CNT/CNF is encapsulated in a hollow cylinder (Figure 5-1a). This outer cylinder is what the author calls an interface, the properties of which can be obtained either by experiments or molecular dynamics. The model further assumes that CNT/CNF is perfectly bonded to the interface and the inclusion (CNT/CNF + interface) is perfectly bonded to the polymer matrix (Figure 5-1b). The analysis for prediction of modulus of nanocomposite is performed in two steps. In the first step, the effective elastic modulus of the inclusion is calculated by considering the inclusion as a long-fiber composite. This is then used as input in the second step where the elastic modulus of the nanocomposite is calculated considering the inclusion and matrix as two phases.

It is assumed that the CNT/CNF’s are straight. Inclusions can be aligned or randomly oriented in the polymer matrix. The properties of the materials of the CNT/CNF, the interface and the matrix are assumed linear.
5.2.  **STEP-1**

Consider a two phase concentric cylinder model shown in Figure 5-1a. In this step, the fiber and interface are aligned. They together can be considered as a composite with an aligned long fiber. The effective modulus of this composite can be calculated using the following three alternative methods:

a) Mechanics method [51]

b) The Mori-Tanaka method [33]

c) An approach that uses rule of mixtures for the longitudinal modulus, and the Poisson’s ratio, and Halpin-Tsai empirical equations for transverse and shear moduli. This approach will be called *Conventional method* in the rest of the thesis [4].

The focus of this thesis is on Mechanics method. Other methods mentioned will be used to compare the results from the first method. Mori-Tanaka [33] yields the stiffness tensor which can be used as input for step-2 but in mechanics and conventional methods,
individual moduli are estimated and the stiffness tensor is formed by assuming transversely isotropic matrix for the inclusion. This assumption is realistic since an aligned fiber exhibits transversely isotropic properties.

5.2.1. MECHANICS METHOD

Assuming the composite material to be macroscopically homogeneous and to obey Hooke’s law, the stress-strain relationships from theory of elasticity as given by Lekhnitskii [31] are,

\[
\begin{align*}
\varepsilon_{xx} &= \left(\frac{1}{E_L}\right) \left[ \sigma_{xx} - \nu_{yx} \sigma_{yy} \right] - \frac{1}{E_L} \sigma_{zz} \\
\varepsilon_{yy} &= \left(\frac{1}{E_T}\right) \left[ \sigma_{yy} - \nu_{yx} \sigma_{xx} \right] - \frac{1}{E_T} \sigma_{zz} \\
\varepsilon_{zz} &= \left(\frac{1}{E_L}\right) \left[ \sigma_{zz} - \nu \left( \sigma_{yy} + \sigma_{xx} \right) \right] \\
\gamma_{yz} &= \left(\frac{1}{G}\right) \tau_{yz} \\
\gamma_{xy} &= \left[ 2(1-\nu_{yx})/E_T \right] \tau_{yz} \\
\gamma_{xz} &= \tau_{xz}/G
\end{align*}
\]

The orientation of axis is shown in Figure 5-3. In Eq. 5-1 above there are five independent elastic constants, which according to [51], [23] are longitudinal modulus, \(E_L\), transverse modulus, \(E_T\), major Poisson’s ratio, \(\nu\), shear modulus, \(G\), and Poisson’s ratio in the x-y plane, \(\nu_{yx}\).

Whitney et al.[51] and Hashin et al [23] have derived equations for the five constants in Eq. 5-1 for conventional, long fiber composites. These studies did not consider the effect of the matrix-fiber interface; they rather modeled the matrix and fiber as two concentric cylinders. The equations derived in [51], [23] can still be applied to
find the five constants for the concentric cylinders representing CNT/CNF and the interface in this study.

In this study, it is assumed that CNT/CNF and interface are isotropic. In the following, the approach by Whitney et al. [51] is summarized.

a) Longitudinal modulus
Consider a cross section of a concentric cylinder composite element as shown in Figure 5-2. The composite element consists of CNT/CNF and interface. Let an axial force be applied to this element so that the axial strain $\varepsilon$ of the composite is constant.

![Figure 5-2 Composite Element (adapted from [51])](image)

Consider an Airy stress function as in Eq. 5-2,

$$
\nabla^4 \phi = \frac{d^4 \phi}{dr^4} + \frac{2}{r} \frac{d^3 \phi}{dr^3} - \frac{1}{r^2} \frac{d^2 \phi}{dr^2} + \frac{1}{r^3} \frac{d \phi}{dr} = 0
$$

5-2
Eq. 5-2 is a form of the Euler differential equation, the solution of which is given by,

\[ \bar{\phi} = c_1 \log r + c_2 r^2 \log r + c_3 r^2 + c_4 \] \hspace{1cm} 5-3

Using a stress function for both CNT/CNF and interface and applying different boundary conditions to solve for the constants in Eq. 5-3 will yield the stresses in the CNT/CNF and the interface. The elastic modulus, \( E_L \), is now obtained by an energy balance.

\[ E_L = \frac{2(v_f - v_i)^2 E_f E_i (1 - V_f) V_f}{E_i (1 - V_f) L' + (L V_f + (1 + V_f)) E_f} + E_i + (E_f - E_i) V_f \] \hspace{1cm} 5-4

where \( L' = 1 - v_i - 2v_i^2 \) and \( L = 1 - v_f - 2v_f^2 \)

The first term of Eq. 5-4 is not significant for most composites [51]. Therefore, the longitudinal modulus can be estimated from the following equation:

\[ E_L = E_i + (E_f - E_i) V_f \] \hspace{1cm} 5-5

The above equation is the rule of mixtures.

b) Major Poisson’s ratio

The major Poisson’s ratio, \( \nu \), can be found from the results of longitudinal modulus. Considering the radial contraction of the composite, the Poisson’s ratio is given by,
\[ v = v_i - \frac{2(v_i - v_f)(1-v_i^2)E_fV_f}{E_i(1-V_f)\ell' + [LV_f + (1+v_f)E_f]} \quad 5-6 \]

where \( \ell' = 1-v_i - 2v_i^2 \) and \( L = 1-v_f - 2v_f^2 \)

c) Transverse modulus

Consider the concentric cylinder model shown in Figure 5-2. The composite model consists of CNT/CNF and interface. In order to find the transverse modulus, a radial pressure is applied to the surface of the composite cylinder. It is also assumed that an axial stress is applied to the composite cylinder such that the axial strain is zero.

The bulk modulus, \( k \), of the cylinder can be found by considering change in volume caused by the pressure,

\[ 1 + \Delta V = (1 + \varepsilon_z)(1 + \varepsilon_y) \quad 5-7 \]

Neglecting second order terms,

\[ \Delta V = \varepsilon_z + \varepsilon_y \quad 5-8 \]

Using stress-strain relationships, the bulk modulus will be,

\[ k = E_L E_T / 2[(1-v_{ys})E_L - 2E_T v^2] \quad 5-9 \]

\( E_T \) needs to be evaluated using Eq. 5-9 which in turn needs the bulk modulus to be evaluated using the known stress-strain relationships.
\[
\sigma'_x = V' \left( \sigma'_f + \sigma'_o \right) \\
\sigma'_y = V' \left( \sigma'_r + \sigma'_o \right) 
\]

Applying the boundary conditions and solving for the constants yield,

\[
k = \frac{\left[ (k_f + G_i)k_f - (k_f - k_i)G_f \right] V_f}{\left[ (k_f + G_i) - (k_f - k_i) \right] V_f}
\]

\[
k_f = \frac{E_f}{2(1 - \nu_f - 2\nu_f^2)} \quad \text{and} \quad k_i = \frac{E_i}{2(1 - \nu_f - 2\nu_f^2)} 
\]

As an approximation, \(\nu_{yx}\), as given by rule of mixtures is assumed to be,

\[
\nu_{yx} = V_f \nu_f + V_i (1 - \nu_f) 
\]

The transverse modulus is obtained by substituting Eqs. 5-5, 5-11 and 5-12 in 5-9 and solving for \(E_T\).

\[
E_T = \frac{2k(1 - \nu_{yx})E_L}{E_L + 4k\nu^2} 
\]

d) Shear modulus

According to Hashin and Rosen [23], for the composite element shown in Figure 5-2, the Cartesian equations of elasticity reduce to,

\[
\nabla^2 u_i = 0 
\]
where \( i = 1, 2, 3 \), and \( \nabla^2 \) is the three-dimensional Laplacian. For the above problem, the simple displacement solution in cylindrical coordinates is given as,

\[
\begin{align*}
    u_i &= u_z = \left( Ar + \frac{B}{r} \right) \cos \theta \\
    u_r &= C \cos \theta \\
    u_\theta &= -C \cos \theta
\end{align*}
\]

where \( A, B, \) and \( C \) are arbitrary constants. After calculating the stresses associated with these solutions and applying boundary conditions the shear modulus can be computed as,

\[
G = \frac{[(G_f + G_i) + (G_f - G_i)V_f]G_i}{[(G_f + G_i) - (G_f - G_i)V_f]}
\]

\[5-16\]

\( E_f \) and \( E_i \) are modulus of CNT/CNF and modulus of interface, \( \nu_f \) and \( \nu_i \), are Poisson’s ratio of CNT/CNF and Poisson’s ratio of interface, \( G_f, G_i \), and \( V_f \) are shear modulus of CNT/CNF, shear modulus of interface and volume fraction of CNT/CNF respectively. The user of this method needs to specify the above elastic constants of the individual phases.
5.2.2. MORI-TANAKA METHOD

The inclusion model described in section 2.1 can be thought of as a nanocomposite with CNT/CNF and interface as two phases. A traditional micro mechanics model, such as the one by Mori-Tanaka (M-T), can be used to represent the effective behavior of nanocomposites. M-T method has been used by wide range of researchers [18]-[42] to predict the stiffness of composites with both aligned and randomly oriented nanofibers. To model the inclusion, we use the model with aligned nanotubes/nanofibers. The M-T method allows the average stress fields and overall effective stiffness of a composite to be determined. Highlighted here are only those expressions from the method that are of interest. For complete derivation of the M-T method, refer to [42]. The basic assumptions and methodology for deriving the stiffness tensor of inclusion are given in [35], [42]. According to [35], [42], the stiffness tensor $C$ for the inclusion is given in Eq. 5-17 with a replacement for matrix $m$ with interface $i$:
\[ C = (V_i C_i + V_r C_r : A) : (V_i I + V_r A)^{-1} \]

\( I \) is the fourth order identity tensor, \( A \) is the fourth order dilute strain concentration tensor that relates average strains \( \varepsilon_r \) and \( \varepsilon_i \),

\[ \varepsilon_r = A : \varepsilon_i \]

\[ A = \left[ I + S : (C_i)^{-1} : (C_r - C_i) \right]^{-1} \]

and \( S \) is the standard Eshelby tensor [16], [18], [42]. Colon between two tensors denotes contraction (inner product) over two indices; the subscripts \( i \) and \( r \) stand for the quantities of the interface and reinforcing phase, respectively, \( V_i \) and \( V_r \) denote the volume fractions, and \( C_i \) and \( C_r \) denote the tensors of elastic moduli of the corresponding phases.

Even though M-T method has been specifically developed for discontinuous fibers, its analytical derivation doesn’t distinguish between long and short fibers, that is, it does not take into consideration the nature of the reinforcement. To apply this method, the interface properties should be assumed isotropic.

The user of this method needs to specify the following input parameters:

a) 5 independent elastic constants if the CNT/CNF is transversely isotropic, as shown in Table 5-1 and 2 independent constants if it is isotropic.

b) The volume fraction of the CNT/CNF or the interface.

c) The elastic modulus and Poisson’s ratio of the interface.
### Table 5-1 Compliance matrices for transversely and isotropic materials for inclusion

**Transversely Isotropic**

(For Fiber oriented in $Z$- direction in Figure 2)

$E_T, \nu_T$-Modulus and Poisson’s ratio in the 1-2 symmetry plane

$E_L, \nu_{LT}, G_{LT}$-Elastic modulus, Poisson’s ratio and shear modulus in 3-direction

\[
\begin{bmatrix}
\frac{1}{E_T} & -\nu_T & -\nu_T & 0 & 0 & 0 \\
-\nu_T & \frac{1}{E_T} & -\nu_T & 0 & 0 & 0 \\
-\nu_T & -\nu_T & \frac{1}{E_T} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2G_{LT}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2G_{LT}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1+\nu_T}{E_T}
\end{bmatrix}
\]

**Isotropic**

$E, \nu$-Elastic modulus and Poisson’s ratio

\[
\begin{bmatrix}
1 & -\nu & -\nu & 0 & 0 & 0 \\
-\nu & 1 & -\nu & 0 & 0 & 0 \\
-\nu & -\nu & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1+\nu & 0 & 0 \\
0 & 0 & 0 & 0 & 1+\nu & 0 \\
0 & 0 & 0 & 0 & 0 & 1+\nu
\end{bmatrix}
\]

Table 5-1 Compliance matrices for transversely and isotropic materials for inclusion

### 5.2.3. CONVENTIONAL APPROACH

A CNT/CNF surrounded by the interface can be considered similar to a conventional composite. Hence the rule of mixtures and Halpin-Tsai empirical relations can be used to find the moduli in different directions, which can then be used to construct a stiffness
matrix for the inclusion. This information will be input in step 2. In contrast to M-T method, Halpin-Tsai method distinguishes between long and short fibers and uses different equations for each type of fiber.

To apply this method, the CNT/CNF and interface properties should be assumed isotropic. According to Eq. 5-1, five independent elastic constants are required but since there are only four, the out-of-plane shear modulus is assumed to be equal to in-plane shear modulus. Now Eq. 5-1 can be rewritten as:

\[
\begin{bmatrix}
\frac{1}{E_T} & -\nu_{TT} & -\nu_{LT} & 0 & 0 & 0 \\
\nu_{TT} & \frac{1}{E_T} & -\nu_{LT} & 0 & 0 & 0 \\
-\nu_{LT} & \nu_{LT} & \frac{1}{E_T} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2G_{LT}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2G_{LT}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{LT}} \\
\end{bmatrix}
\]

5-20

The following equations estimate moduli in different directions. The rule of mixtures is used to estimate the longitudinal modulus:

\[
E_L = E_f V_f + E_i V_i
\]

5-21
where $E_f$, $V_f$, $E_i$, $V_i$ are the moduli of elasticity and volume fractions of the fiber and interface materials, respectively.

The transverse modulus, $E_T$, is estimated using Halpin-Tsai empirical relations. As per Halpin and Tsai the transverse modulus is:

$$
\frac{E_T}{E_i} = 1 + \xi \eta V_f
$$

where, $$\eta = \frac{\left(\frac{E_f}{E_i}\right)^{-1}}{\left(\frac{E_f}{E_i}\right)^{+} + \xi}$$

Constant, $\xi$ is equal to 2 for fibers with circular or square cross-section, and it is equal to $2 \frac{a}{b}$ for fibers with rectangular cross-section. $\frac{a}{b}$ is the rectangular cross-section aspect ratio, where dimension $a$ is taken in the direction of loading.

The shear modulus ($G_{LT}$) is also estimated by an empirical relation by Halpin-Tsai:

$$
\frac{G_{LT}}{G_i} = 1 + \xi \eta V_f
$$

where $$\eta = \frac{\left(\frac{G_f}{G_i}\right)^{-1}}{\left(\frac{G_f}{G_i}\right)^{+} + \xi}$$

$\xi = 1$ (Suggested by Halpin & Tsai)

The three Poisson’s ratios can be calculated from the following equations:

The Poisson’s ratio in the x-y symmetry plane can be obtained by solving the equation for the definition of the shear modulus:

$$
\nu_T = \frac{E_T}{2G_{LT}} - 1
$$
The Poisson’s ratio in the 3-direction is given by:

\[ \nu_{LT} = \nu_f V_f + \nu_i V_i \]

Also,

\[ \frac{V_{IL}}{E_i} = \frac{V_{LT}}{E_L} \]

Once the compliance matrix is formed, the stiffness matrix is obtained by inversion,

\[ \text{Stiffness Matrix} = \left[ \text{Compliance Matrix} \right]^{-1} \]

The user of Halpin-Tsai method needs to specify the following input parameters:

a) Two independent constants (modulus and Poisson’s ratio) since the CNT/CNF is assumed isotropic.

b) The volume fraction of fiber or the interface.

c) The elastic modulus and Poisson’s ratio of the interface.

The preceding section described three alternative methods that can be used for step-1 of the encapsulated inclusion model. The following section describes step-2 of the same model where in M-T method has been used.

5.3. STEP-2

After the inclusion stiffness matrix has been computed, to predict the overall stiffness of the nanocomposite (inclusion + matrix), the M-T micromechanical model is used for predicting mechanical behavior of nanocomposites [18], [42]. This model is more suitable than the Halpin-Tsai model for nanocomposites, because the later model assumes long fibers. For a nanocomposite with inclusions aligned in a polymer matrix, the
stiffness matrix is represented by equations 5-17 - 5-19 with subscript \( i \), for the interface replaced by subscript \( m \) for the matrix. For a nanocomposite with randomly oriented inclusions, the stiffness tensor \( C \) is given by:

\[
C = (V_m C_m + V_r \{C_r : A\}) : (V_m I + V_r \{A\})^{-1}
\]

The curly brackets \( \{ \} \) represent the orientational average of the quantity within the brackets [42] (average over special orientations) and \( V_r \) represent volume fraction of the inclusion (CNT/CNF + matrix).

### 5.4. NUMERICAL EXAMPLES

**Problem**: A nanocomposite with randomly oriented CNFs is analyzed here. In step-1, the inclusion stiffness matrix is computed using Mechanics (Eq. 5-1), M-T (Eq. 5-17) and Conventional (Eq. 5-20) methods. In step-2, the M-T method (Eq. 5-26) that accounts for random orientations of the inclusions is applied.

Six cases are studied in which the Mechanics, M-T and Conventional approaches are employed in step-1. These results are compared with those obtained by ignoring the effect of the interface, to assess the effect of the interface on the overall composite modulus. These analytical results are also compared with published experimental results [6].

#### 5.4.1. CASE 1: MECHANICS METHOD IN STEP-1

The CNT/CNF is isotropic with 2 independent elastic constants.

<table>
<thead>
<tr>
<th>( E_f )</th>
<th>Elastic modulus of CNT/CNF</th>
<th>200 GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu_f )</td>
<td>Poisson’s ratio of CNT/CNF</td>
<td>0.3</td>
</tr>
</tbody>
</table>
The properties of the interface can be obtained using a molecular dynamics model or experiments. In this example, we assume that the properties of the interface are same as those of the matrix. The volume fraction of the interface was assumed 0.1. The interface properties are presented below.

<table>
<thead>
<tr>
<th>$v_i$</th>
<th>Poisson’s ratio of interface</th>
<th>0.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_i$</td>
<td>Young’s modulus of interface</td>
<td>2 GPa</td>
</tr>
<tr>
<td>$V_i$</td>
<td>Volume fraction of interface</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The matrix properties are as follows:

<table>
<thead>
<tr>
<th>$v_m$</th>
<th>Poisson’s ratio of matrix</th>
<th>0.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_m$</td>
<td>Young’s modulus of matrix</td>
<td>2 GPa</td>
</tr>
</tbody>
</table>

First Eq. 5-1 was applied, which yields the stiffness matrix of inclusion. Then Eq. 28 was applied to determine the stiffness matrix of the overall CNT/CNF composite. Figure 5-4 shows the modulus of elasticity of the composite as a function of the volume fraction of the inclusion.
It is observed that when the volume fraction of the inclusion is zero, then, as expected, the modulus of the composite is equal to the modulus of the matrix (Figure 5-4). When the volume fraction of the inclusion is one, the modulus of the composite is equal to the directional average of the modulus of the CNT/CNF. The modulus of the composite, when the effect of the interface is taken into account is considerably lower than that when the effect of the interface is ignored. For example, for a volume fraction of 0.08 the modulus of the composite is 44.7% lower than that when the effect of the interface is ignored.

The effect of the volume ratio of the inclusion is linear for volume fractions in the range from 0 to 0.2 (Figure 5-5). The modulus increases at a higher rate for larger volume
fraction coefficients. However this result will change when one accounts for agglomeration in fibers for higher volume fractions.

It is also observed that the model predictions are much higher than experimental measurements. This can be due to deficiencies in the model of the interface, errors in the values of the interface parameters, and agglomeration of the fibers.

![Variation of E with Volume fraction of inclusion using Mechanics in step-1](image)

**Figure 5-5** Variation of E with Volume fraction of inclusion using Mechanics in step-1

### 5.4.2. CASE 2: M-T METHOD IN STEP-1

The CNT/CNF is transversely isotropic with 5 independent elastic constants. These elastic constants \((k, n, l, m, and p)\) are known as Hill’s elastic moduli [42]. The stiffness matrix can be determined using these constants as shown below:
\[
\begin{bmatrix}
  k + m & l & l & 0 & 0 & 0 \\
l & n & k - m & 0 & 0 & 0 \\
l & k - m & n & 0 & 0 & 0 \\
0 & 0 & 0 & \sqrt{\frac{n - l}{2}} & 0 & 0 \\
0 & 0 & 0 & 0 & p & 0 \\
0 & 0 & 0 & 0 & 0 & p
\end{bmatrix}
\]

As in case 1, we assume that the properties of the interface are same as those of the matrix. The volume fraction of the interfaced was assumed 0.1. The interface properties are presented below.

| \( k \) | Plane-strain bulk modulus normal to the CNT/CNF direction | 30 GPa  |
| \( n \) | Uniaxial tension modulus in CNT/CNF direction | 450 GPa  |
| \( l \) | Associated cross modulus | 10 GPa  |
| \( m, p \) | Shear moduli in planes normal and parallel to the CNT/CNF direction | 1 GPa  |

The matrix properties are as follows:

| \( v_i \) | Poisson’s ratio of interface | 0.3 |
| \( E_i \) | Young’s modulus of interface | 2 GPa  |
| \( V_i \) | Volume fraction of interface | 0.1 |

| \( v_m \) | Poisson’s ratio of matrix | 0.3 |
| \( E_m \) | Young’s modulus of matrix | 2 GPa  |

First Eq. 5-17 was applied, which yields the stiffness matrix of inclusion. Then Eq. 5-28 has been applied to determine the stiffness matrix of overall CNF composite. Figure 6 shows the modulus of elasticity of the composite as a function of the volume fraction of the inclusion.
It is observed that when the volume fraction of the inclusion is zero, then the modulus of the composite is equal to the modulus of the matrix (Figure 5-6). When the volume fraction of the composite is one, the modulus of the composite is equal to the directional average of the modulus of the fiber. The modulus of the composite, when the effect of the interface is taken into account is considerably lower than that when the effect of the interface is ignored. For example, for a volume fraction of 0.08 the modulus of the composite is 8.2% lower than that when the effect of the interface is ignored.

The effect of the volume ratio of the inclusion is linear for volume fractions in the range from 0 to 0.2. The modulus increases at a higher rate for larger volume fraction coefficients. However this result will change when one accounts for agglomeration in fibers for higher volume fractions.

**Figure 5-6 Variation of composite modulus with volume fraction of inclusion using M-T in step-1**
It is also observed that the model predictions are much higher than experimental measurements. This can be due to deficiencies in the model of the interface, errors in the values of the interface parameters, and agglomeration of the fibers.

5.4.3. CASE 3: CONVENTIONAL METHOD IS USED IN STEP-1

Here the Conventional method is used to estimate the elastic moduli of the inclusion in step 1 instead of the Mechanics or M-T methods. The CNT/CNF is assumed isotropic. Two independent elastic constants are needed to specify the CNT/CNF properties in this case. These are shown below.

<table>
<thead>
<tr>
<th>$E_f$</th>
<th>Modulus of CNT/CNF</th>
<th>200 GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu_f$</td>
<td>Poisson’s ratio</td>
<td>0.3</td>
</tr>
</tbody>
</table>

The interface and matrix properties are the same as in case 1.

Figure 5-7 shows the variation of the modulus of the composite with the volume fraction of the inclusion. When the volume fraction of the inclusion is one and there is no interface (the CNT/CNF is perfectly bonded to the matrix), the overall composite modulus equals that of the CNT/CNF (which is 200 GPa). The modulus of the composite, when the effect of the interface is taken into account is considerably lower than that when the effect of the interface is ignored. For example, for a volume fraction of 0.08 the modulus of the composite is 7.6% lower than that when the effect of the interface is ignored.
5.4.4. CASE 4: COMPARISON OF METHODS THAT USE MECHANICS, M-T AND CONVENTIONAL METHODS IN STEP-1

Here, a comparison is made between moduli predicted by the developed encapsulated approach using the three methods in step-1 (Mechanics, M-T and Conventional methods).

The CNT/CNF and the matrix properties are the same as in case 4. The interface properties are as follows:

\[
\begin{array}{|c|c|c|}
\hline
i & v_i & Poisson’s ratio of interface \\ 
& E_i & Young’s modulus of interface \\ 
& V_i & Volume fraction of interface \\ 
\hline
& 0.3 & 2 \text{ GPa} \\ 
& 0.1 & \\ 
\hline
\end{array}
\]
Figure 5-8 Comparison of Mechanics, M-T and Conventional methods
Figure 5-8 and Figure 5-9 compare different methods for calculating stiffness matrix for inclusion in step-1 for different ranges. The difference in the results of the three methods can be attributed to the following:

Figure 5-8 shows that the three methods yield significantly different results. However, as Figure 5-9 indicates, in practical applications where the volume fraction ranges from 0 to 0.2, the results of the three methods are close to each other.

The estimates of the elastic modulus of the composite from the conventional approach are higher than those of the M-T method. The reason is that the M-T method assumes discontinuous short fibers in step 1 (estimation of the modulus of the inclusion), while the Conventional method assumes long fibers in step 1. The conventional method is more realistic for the interface than the M-T method (Figure 5-1a).
The Mechanics method underestimates the elastic modulus compared to the conventional method that uses Halpin-Tsai empirical equations. The authors believe that the results of the Mechanics method are more accurate than those of the conventional method because the Mechanics method is based on first principles while Halpin-Tsai method is empirical.

Because the MT method is not suitable for long fiber composites and because the model of the inclusion is a long fiber composite, the Mechanics method should be the most suitable of the three methods.

5.4.5. POST BUCKLING RESPONSE OF A RECTANGULAR GRAPHITE-EPoxy PLATE

The computed stiffness matrix of nanocomposite with interface, Eq. 5-28, will be used as input for failure analysis model developed by Hammitt [21]. The same example problem presented in section 4.3 and Pilla et al.[35] will be solved for load-deflection history.

The post buckling response of a flat rectangular graphite-epoxy plate was analyzed. Figure 5-10 gives the properties and geometry (Source: Hammitt [21]) of the plate. The nanofibers/nanotubes are randomly oriented in the polymer matrix. The total applied load is 2100 N.
Figure 5-10 Properties of Graphite Epoxy Plate (Source: Hammitt [21])

Nano Composite

\[ E_f = 200000 \text{ MPa} \]
\[ E_m = 1900 \text{ MPa} \]
\[ v_f = 0.3 \]
\[ v_m = 0.3 \]
\[ V_f = 5\% - 10\% \]
\[ V_i = 0.3 \]
\[ E_i = 2000 \]
\[ V_i = 0.9 \]

Figure 5-11 shows the post buckling response for plates with volume fractions of nanofiber/nanotube of 5\% and 10\%. As expected, the plate with a higher volume fraction of fiber exhibits greater strength than the plate with less fiber.
CHAPTER 6. PROBABILISTIC AND RELIABILITY ANALYSIS OF NANOCOMPOSITES

6.1. INTRODUCTION

There is large uncertainty in the properties of CNT/CNF’s because it is difficult to measure these properties. A methodology has been developed in this chapter that accounts for the uncertainties and variability in the moduli of the constituent materials of a CNT/CNF composite and computes the probability density function of overall composite modulus.

In addition to uncertainty in properties of phase materials, there is variation found in manufacturing environment and processes which induces variation in the geometry of the structure. Due to these factors the material has many imperfections even before it is ready for design. Therefore, all these imperfections, uncertainties should be taken into consideration while designing a structure. Such a design is known as reliability based design for which it is very important to know the reliability of the structure. This chapter will focus on finding the probability of failure of a nanocomposite plate. The input for the reliability analysis is given by probabilistic analysis. The methodology for reliability analysis has been developed by Hammitt [21] and is based on well established reliability theories.
6.2. PROBABILISTIC ANALYSIS

There is large uncertainty in the properties of CNT/CNF’s because it is difficult to measure these properties. A methodology has been developed that accounts for the uncertainties and variability in the moduli of the constituent materials of a CNT/CNF composite and computes the probability density function of overall composite modulus.

6.2.1. APPROACH

First we need to estimate the probability density function (PDF) of moduli of the constituent materials of a nanocomposite. The PDF of modulus of CNT/CNF can be estimated by using the bounds given by the user by assuming a standard distribution. For the matrix and interface, the modulus is specified either in terms of a mean value with an associated standard deviation or in terms of lower and upper bounds similar to CNT/CNF. It is assumed to follow some standard distribution to compute the PDF.

Once the PDFs of moduli of constituent materials are established, Monte Carlo simulation is used to generate $n$ sample values of modulus of CNT/CNF, interface and matrix. For each value, the modulus of composite is calculated using micromechanical model described in sections 5.2 and 5.3 of this study. Once all the $n$ modulus values of composite are determined, a standard PDF such as uniform, normal or Weibull, can be fit to the results. This PDF can be used for reliability analysis of nanocomposites [21], [35]. The user of this method needs to specify the following input parameters:

a) Lower and upper bounds for the modulus of CNT/CNF.

b) Lower and upper bounds or the mean value and standard deviation of the moduli of the interface and matrix.
c) Number of Monte Carlo simulations.

d) Poisson’s ratio of the CNT/CNF, interface and matrix.

6.2.2. ESTIMATING THE PDF OF THE MODULUS OF CNT/CNF, INTERFACE AND MATRIX

We assume that the modulus of CNT/CNF, interface and matrix to follow a uniform distribution [38]. The probability density function is given in Eq. 6-1

\[ f(x) = \frac{1}{B - A} \quad \text{for} \quad A \leq x \leq B \]  

6-1

where \( A \) is the location parameter and \( B - A \) is the scale parameter.

The case where \( A = 0 \) and \( B = 1 \) is called the standard uniform distribution. The equation for the standard uniform distribution is given in Eq. 6-2.

\[ f(x) = 1 \quad \text{for} \quad 0 \leq x \leq 1 \]  

6-2

6.3. NUMERICAL EXAMPLES

**Problem:** A nanocomposite with randomly oriented inclusions (CNT/CNF + interface) with the following properties is analyzed here:

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_f ) (lower)</td>
<td>Lower bound of modulus of CNT/CNF</td>
<td>150000 MPa</td>
</tr>
<tr>
<td>( E_f ) (upper)</td>
<td>Upper bound of modulus of CNT/CNF</td>
<td>250000 MPa</td>
</tr>
<tr>
<td>( V_f )</td>
<td>Volume fraction of CNT/CNF</td>
<td>0.9</td>
</tr>
<tr>
<td>( V_r )</td>
<td>Volume fraction of inclusion</td>
<td>0.05</td>
</tr>
<tr>
<td>( E_m ) (lower)</td>
<td>Lower bound of modulus of matrix</td>
<td>1850 MPa</td>
</tr>
<tr>
<td>( E_m ) (upper)</td>
<td>Upper bound of modulus of matrix</td>
<td>1950 MPa</td>
</tr>
</tbody>
</table>
Figure 6-1 and Figure 6-2 show the histograms of the modulus of the composite with interface (step-1, Mechanics method-section 5.2.1 and step-2, Mori-Tanaka method-section 5.3) and without interface (Mori-Tanaka method-section 4.2.2) respectively. These results were obtained using 10,000 simulations. As mentioned earlier, for a nanocomposite with interface, the Mechanics approach is believed to be more realistic than the Conventional and M-T methods. The descriptive statistics of the data for the two cases (with and without interface respectively) is shown in Table 6-1 and Table 6-2.

### Table 6-1: Descriptive Statistics for data of nanocomposite modulus considering the effect of interface

<table>
<thead>
<tr>
<th>Column1(With Interface)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>3542.822</td>
</tr>
<tr>
<td>Median</td>
<td>3543.321</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>225.227</td>
</tr>
<tr>
<td>Kurtosis</td>
<td>-1.1569</td>
</tr>
<tr>
<td>Skewness</td>
<td>-0.009</td>
</tr>
<tr>
<td>Minimum</td>
<td>3097.21</td>
</tr>
<tr>
<td>Maximum</td>
<td>3985.435</td>
</tr>
</tbody>
</table>

### Table 6-2: Descriptive Statistics for data of nanocomposite modulus not considering the effect of interface

<table>
<thead>
<tr>
<th>Column2(Without Interface)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>3767.42</td>
</tr>
<tr>
<td>Median</td>
<td>3765.11</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>252.407</td>
</tr>
<tr>
<td>Kurtosis</td>
<td>-1.148</td>
</tr>
<tr>
<td>Skewness</td>
<td>0.0105</td>
</tr>
<tr>
<td>Minimum</td>
<td>3283.352</td>
</tr>
<tr>
<td>Maximum</td>
<td>4254.323</td>
</tr>
</tbody>
</table>
Figure 6-1 Histogram of Modulus of Composite with interface (The modulus is expressed in MPa)
Qualitatively, the histograms seem to follow uniform distribution. This can be attributed to the fact that CNT/CNF which dominates in randomness (Figure 6-3) was modeled with uniform distribution.

The importance of the uncertainties can be assessed from Figure 6-3. The dashed bars in this figure show the variance in the modulus of the composite when each of the three random variables becomes deterministic, while the gray bars show the variance in the modulus when all three variables are random. The larger the reduction in the variance when a variable is assumed deterministic, the more important that variable is. Clearly, the uncertainty in the CNT/CNF modulus dominates. If this uncertainty were eliminated, then the uncertainty in the composite modulus would be greatly reduced. This shows the importance of modeling the uncertainty in the CNT/CNF modulus.
6.4. RELIABILITY ANALYSIS

The probabilistic analysis performed in section 6.2 yields mean and standard deviation of modulus of nanocomposite based on the PDF of nanofiber/nanotube, matrix and interface modulus. As stated in section 1.2.3, this can be taken as input for reliability analysis of nanocomposite plates.

The output from the probabilistic analysis, mean and standard deviation of modulus of nanocomposite, will be used as input to the reliability analysis model presented by Hammitt [21]. Figure 6-4 shows the flow chart that connects the probabilistic, micromechanics and reliability analysis models for nanocomposite with interface. If the interface is neglected then the PDF of modulus of interface is neglected and also
correspondingly in the micromechanics method instead of two-step approach (sections 5.2 and 5.3), direct Mori-Tanaka method as explained in section 4.2 is applied.

```
PDF of moduli of nanofiber/nanotube, matrix, interface

Generate N random numbers for moduli

Set counter=1

Micromechanical Model

Volume fraction of phase materials

Is Counter=N

No

counter = counter + 1

Yes

Compute Mean and Standard Deviation of Modulus of nanocomposite

Failure and Reliability Analysis Model

Probability of failure
```

Figure 6-4 Flow chart that connects probabilistic and reliability analysis models
6.5. NUMERICAL EXAMPLES

The same example problem presented in section 4.3 is considered here, with the modulus of nanocomposite, load factor, yield strength and imperfection as random variables. For nanocomposite (considering the CNT/CNF-matrix interface), the inclusion (CNT/CNF + interface) is assumed to be randomly oriented in polymer matrix and for nanocomposite without considering the effect of interface, CNT/CNF is believed to be randomly dispersed in polymer matrix. Figure 6-5 shows the geometry (Source: Hammitt [21]) and input parameters for both the problems. Table 6-3 shows the random variable $E$ properties. Other random variable properties are given in Hammitt [21]. The maximum allowable displacement was set at 42 mm and the maximum allowable strain was 0.5 mm/mm.

![Geometry and input parameters for graphite-epoxy plate](Source: Hammitt [21])

<table>
<thead>
<tr>
<th>Property</th>
<th>Mean</th>
<th>SD</th>
<th>Variable Type</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (with interface)</td>
<td>3543</td>
<td>225</td>
<td>normal</td>
<td>Mpa</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>3767</td>
<td>252</td>
<td>normal</td>
<td>Mpa</td>
</tr>
</tbody>
</table>

Table 6-3 Random input variables
The results of the analysis for nanocomposites with interface and without interface are shown in Figure 6-6 and Figure 6-7 respectively. The vertical axis represents the probability of failure, and the horizontal axis represents various analytical and simulation techniques. Good agreement is observed among the methods, and some variation is expected due to the fact that each of them gives only an approximation of the failure probability. Mode 1 (failure due to excessive deflection) is more important than Mode 2 (failure due to straining). Note that the computed probabilities of failure are high by most standards, and would not be acceptable in practice. They are acceptable, however, for the academic purpose of verifying the methodology.

![Figure 6-6 Probability of failure computed by Monte Carlo simulation and FORM (with interface)](image-url)

Figure 6-6 Probability of failure computed by Monte Carlo simulation and FORM (with interface)
The histograms of Young’s modulus, $E$, in section 6.3 suggest that the Young’s modulus of nanocomposite, $E$, follows a uniform distribution. However, the results of reliability analysis in Table 6-4 show that if $E$ is assumed to follow a normal distribution the failure probabilities of the two failure modes do not change significantly compared to the estimates corresponding to a uniform distribution.

<table>
<thead>
<tr>
<th>Property</th>
<th>Method</th>
<th>Mode 1 P(f)</th>
<th>Mode 2 P(f)</th>
<th>Variable Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 100</td>
<td>0.33</td>
<td>0.31</td>
<td>Normal</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 500</td>
<td>0.34</td>
<td>0.34</td>
<td>Uniform</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 1000</td>
<td>0.304</td>
<td>0.322</td>
<td>Normal</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 1000</td>
<td>0.3</td>
<td>0.32</td>
<td>Uniform</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 500</td>
<td>0.306</td>
<td>0.333</td>
<td>Normal</td>
</tr>
<tr>
<td>$E$ (without interface)</td>
<td>MC (IS) 1000</td>
<td>0.31</td>
<td>0.332</td>
<td>Uniform</td>
</tr>
</tbody>
</table>

MC (IS) X – Monte Carlo Simulation with Importance Sampling for X random values

Table 6-4 Comparison of probability of failure for uniform and normal distributions of $E$

6.5.1. COMPARISON OF PROBABILITY OF FAILURES OF NANOCOMPOSITE PLATES WITH AND WITH OUT INTERFACE

In this section a comparison is made for the probability of failure obtained by reliability analysis of nanocomposite plates with and without interface. The same
example shown in Figure 6-5 is solved. Figure 6-8 and Figure 6-9 show the comparisons for two different failure modes. Note that failure mode 1 is failure due to excessive deflection and Mode 2 is failure due to straining.

![Failure by Mode-1](image)

**Figure 6-8 Comparison of probability of failure of nanocomposite plates with and without interface for failure mode - 1**

![Failure by Mode-2](image)

**Figure 6-9 Comparison of probability of failure of nanocomposite plates with and without interface for failure mode - 2**

In either failure modes, the probability of failure of nanocomposite plates without considering the effect of interface is lower than the probability of failure of
nanocomposite with interface. Because the reinforcement is not rigidly connected to the matrix, neglecting the flexibility of the interface could result in underestimating the probability of failure of the plate.
CHAPTER 7. CONCLUSION

7.1. CONCLUDING REMARKS

A model for calculating the stiffness matrix of nanocomposites considering the effect of the CNT/CNF-matrix interface has been developed and presented. Moreover, a probabilistic model that predicts the probability distribution of the stiffness of nanocomposites has been developed. These models have been integrated with a method for failure analysis of structures, developed by Hammitt [21], into a methodology for predicting the load-deflection history and probability of failure of plate structures made of conventional and nanocomposite materials.

The methodology presented in this thesis incorporates following components:

1. Micromechanics/Constitutive model of Conventional and Nano Composites

Methods have been presented for stiffness analysis of conventional composites. A model has been adapted from previous studies for nanocomposites. This model assumes a rigid connection between the CNT/CNF and matrix. Because the interface between the CNT/CNF and the matrix is flexible, an encapsulated inclusion model has been developed to account for this flexible interface. For this purpose, three different methods (mechanics, conventional and Mori-Tanaka) have been used. The results of this interface model have been compared with
results of the method that neglects the effect of the interface (that is, the method that assumes a rigid connection between CNT/CNF and matrix). When accounting for the effect of the interface, the elastic modulus of the nanocomposite decreases considerably. This indicates that it could be important to account for the effect of the CNT/CNF-matrix interface on the properties of the nanocomposite. For small values (less than 0.2) of the volume fraction of the inclusion the modulus of the interface increases linearly with the volume fraction of the inclusion. However, this conclusion can change if the effect of agglomeration is accounted for.

The properties predicted by the micromechanics model are used as input for the deterministic analysis model developed by Hammitt [21] that calculates the load-deflection history of plates.

2. Model for Probabilistic Analysis of Nanocomposites

A methodology has been established and demonstrated by assessing the uncertainty in the modulus of a nanocomposite due to the uncertainty in the moduli of the constituent phases of the nanocomposite. Sensitivity analysis of nanocomposite modulus to the moduli of the constituent materials has been also performed. In the particular example considered the modulus of the composite was found to be sensitive only to the uncertainty in the CNT/CNF modulus. The moduli of the interface and matrix can be considered to be deterministic. The results of the probabilistic model are inputs to the model presented by Hammitt [21] for estimating the probability of failure of plates.
7.2. RECOMMENDATIONS FOR FUTURE WORK

The following are the recommendations for future work:

- The encapsulated inclusion model presented in this study assumes the properties of interface to be supplied by the user of the program. These can be obtained either by molecular dynamics analysis or experiments. When such results become available they should be input to the encapsulated inclusion model. The predictions of the model should be compared with published analytical and experimental results.

- In step-1 of the encapsulated inclusion model, methods based on theory of elasticity or semi empirical methods are employed. A numerical approach, such as finite element method, can be used to validate the results of these methods.

- The interface is assumed to surround the CNT/CNF only at the circumference. The approach can be modified to encapsulate the CNT/CNF all around including the circular ends.

- The interface properties are assumed to be linear elastic. The encapsulated inclusion model can be modified to account for nonlinearity in the interface properties.

- Spatial variability, that is, variation from point to point in the constituent materials could be important. The importance of the spatial variability should be assessed and the model could be extended to account for this variability.
APPENDIX I: User Manual for Fortran 90
Program COMPOSITETESTING2

COMPOSITETESTING2

Program for Stiffness and Probabilistic Analysis of Conventional and Nano Composites

Srikanth Pilla

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Introduction

COMPOSITETESTING2 is a program, written in Fortran 90, for Stiffness and Probabilistic Analysis of Conventional and Nano Composites. The program can be run in two modes:

1. Stiffness Analysis, which computes the stiffness matrix of conventional and nano composites.
2. Probabilistic analysis using Monte Carlo simulation which computes the mean and standard deviation of stiffness of nanocomposites.

Conventional composite stiffness is predicted for single and multiple laminae. Nanocomposite stiffness is predicted with and without considering interface between reinforcement and matrix.

Input File

The input to the program is provided by input file. The file consists of a number of lines, or cards, which provide the parameters for some aspect of the program. The input file is summarized below:

<table>
<thead>
<tr>
<th>compinp</th>
<th>Input file, which contains information about the properties of individual phase materials of conventional and nanocomposite material and their randomness</th>
</tr>
</thead>
</table>

Parameters

(Model 1=uni. 2=s.f. 3=n.f.)

//Model that defines which composite is being considered//

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>represents conventional unidirectional long fiber composite</td>
</tr>
<tr>
<td>2</td>
<td>represents conventional unidirectional/random short fiber composite</td>
</tr>
<tr>
<td>3</td>
<td>represents unidirectional/random nanocomposite</td>
</tr>
</tbody>
</table>
### Probabilistic vs Deterministic Analysis

- **Deterministic analysis**, predicts stiffness matrix of conventional and nano composites
- **Probabilistic analysis**, predicts the randomness of nanocomposite modulus considering uncertainty and variability in phase material properties

### Uncertainty Values for Nanocomposite

<table>
<thead>
<tr>
<th>NR</th>
<th>Number of Monte Carlo simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-lowf</td>
<td>Lower value of nanocomposite reinforcement modulus</td>
</tr>
<tr>
<td>B-upf</td>
<td>Upper value of nanocomposite reinforcement modulus</td>
</tr>
<tr>
<td>A-lowm</td>
<td>Lower value of nanocomposite matrix modulus</td>
</tr>
<tr>
<td>B-upm</td>
<td>Upper value of nanocomposite matrix modulus</td>
</tr>
<tr>
<td>A-lowi</td>
<td>Lower value of nanocomposite interface modulus</td>
</tr>
<tr>
<td>B-upi</td>
<td>Upper value of nanocomposite interface modulus</td>
</tr>
</tbody>
</table>

### Random Values for Short Fiber Composite

- **Random**: ‘0’ represents short fibers are aligned, ‘1’ represents short fibers are randomly oriented
- **Fiber Len**: Length of short fiber (Halpin-Tsai model)
- **Fiber Dia**: Diameter of short fiber (Halpin-Tsai model)

### Values for Long Fiber Composite

<table>
<thead>
<tr>
<th>Ef</th>
<th>modulus of fiber</th>
</tr>
</thead>
<tbody>
<tr>
<td>Em</td>
<td>Modulus of matrix</td>
</tr>
<tr>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>Vf</td>
<td>volume fraction of fiber</td>
</tr>
<tr>
<td>Vm</td>
<td>volume fraction of matrix</td>
</tr>
<tr>
<td>fibers</td>
<td>cross-section of fibers ‘0’ represents circular cross-section ‘1’ represents rectangular cross-section</td>
</tr>
<tr>
<td>aspect</td>
<td>aspect ratio of fibers ((l/d)) (l) - length of long fibers (d) – diameter of long fibers (circular cross-section)</td>
</tr>
<tr>
<td>poisson's of fiber</td>
<td>Poisson’s ratio of fiber</td>
</tr>
<tr>
<td>poisson's of matrix</td>
<td>Poisson’s ratio of matrix</td>
</tr>
</tbody>
</table>

\[\text{ep} \quad \text{ez} \quad \text{vpz} \quad \text{gzp} \quad \text{vp}\]

//5 elastic properties of nanocomposite reinforcement if the reinforcement is considered to be transversely isotropic//

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ep</td>
<td>Young's modulus of nanofiber in x-y symmetry plane</td>
</tr>
<tr>
<td>ez</td>
<td>Young's modulus of nanofiber in z-direction</td>
</tr>
<tr>
<td>vpz</td>
<td>Poisson’s ratio in z-direction</td>
</tr>
<tr>
<td>gzp</td>
<td>Shear modulus in z-direction</td>
</tr>
<tr>
<td>vp</td>
<td>Poisson’s ratio of nanofiber in x-y symmetry plane</td>
</tr>
</tbody>
</table>

\[\text{iso} \quad \text{intface} \quad \text{option} \quad \text{orientation}\]

//values for nanocomposite//

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>iso</td>
<td>‘0’ represents nanofiber is transversely isotropic ‘1’ represents nanofiber is isotropic</td>
</tr>
<tr>
<td>intface</td>
<td>‘0’ represents interface doesn’t exist i.e. rigid connection between nanofiber and matrix ‘1’ represents interface exists between nanofiber and matrix</td>
</tr>
<tr>
<td>option</td>
<td>‘1’ represents nanofibers are straight + aligned ‘2’ represents nanofibers are straight + random</td>
</tr>
<tr>
<td>orientation</td>
<td>‘2’ represents nanofibers are oriented in 2D direction ‘3’ represents nanofibers are oriented in 3D direction</td>
</tr>
<tr>
<td>-------------</td>
<td>---------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>em</td>
<td>Modulus of nanocomposite matrix</td>
</tr>
<tr>
<td>vm</td>
<td>Poisson’s ratio of nanocomposite matrix</td>
</tr>
<tr>
<td>ef</td>
<td>Modulus of nanofibers</td>
</tr>
<tr>
<td>vf</td>
<td>Poisson’s ratio of nanofibers</td>
</tr>
<tr>
<td>fr</td>
<td>Volume fraction of nanofibers</td>
</tr>
<tr>
<td>vf1</td>
<td>Volume fraction of nanofiber (when interface is considered)</td>
</tr>
<tr>
<td>ei</td>
<td>Modulus of nanocomposite interface</td>
</tr>
<tr>
<td>nui</td>
<td>Poisson’s ratio of nanocomposite interface</td>
</tr>
</tbody>
</table>

//Conventional composite lamina properties//

<table>
<thead>
<tr>
<th>Number of Plies</th>
<th>Total number of plies that make up the material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total thickness of laminate</td>
<td>Sum of all ply thickness values</td>
</tr>
<tr>
<td>Symmetric?</td>
<td>‘1’ represents the arrangement of plies is symmetric ‘2’ represents the arrangement of plies is not symmetric</td>
</tr>
</tbody>
</table>
The information of all plies is then individually given under this ‘tag’ in the following order:

<table>
<thead>
<tr>
<th>Ply number</th>
<th>thickness</th>
<th>angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.14</td>
<td>45</td>
</tr>
<tr>
<td>2</td>
<td>0.14</td>
<td>30</td>
</tr>
<tr>
<td>3</td>
<td>0.08</td>
<td>15</td>
</tr>
</tbody>
</table>

If the plies are symmetric then only half of them are entered.

Output Files

Several files are written as output during a COMPOSITETESTING2 analysis.

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>compout</td>
<td>Main output file, generated by stiffness analysis. Contains the stiffness matrix of conventional or nano composite.</td>
</tr>
<tr>
<td>Es</td>
<td>Generated by probabilistic analysis. Contains random values of nanocomposite modulus (nanofibers are randomly oriented).</td>
</tr>
<tr>
<td>Elong</td>
<td>Generated by probabilistic analysis. Contains random values of nanocomposite longitudinal modulus (nanofibers are aligned).</td>
</tr>
<tr>
<td>Etrans</td>
<td>Generated by probabilistic analysis. Contains random values of nanocomposite transverse modulus (nanofibers are aligned).</td>
</tr>
</tbody>
</table>

Running the Program COMPOSITETESTING2

The program is compiled, built and executed as any regular fortran 90 program.

Post processing the Results

Though no post processing is built into the program, it is recommended that a spreadsheet program such as Microsoft Excel be used to plot the data.
# Listing of Program Source Files for COMPOSITETESTING2

<table>
<thead>
<tr>
<th><strong>Main Program</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Compositetesting2.f90</td>
<td>Main program.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Conventional Composite</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>readdata.f90</td>
<td>Reads input file and allocates/assigns variables appropriately.</td>
</tr>
<tr>
<td>formD.f90</td>
<td>Forms constitutive matrix for composite plane stress plate element.</td>
</tr>
<tr>
<td>input.f90</td>
<td>Computes properties of a single ply</td>
</tr>
<tr>
<td>Qforaply.f90</td>
<td>Forms constitutive matrix for a single ply</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Nanocomposite</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>alignedrandom.f90</td>
<td>Computes the stiffness matrix of nanocomposite in which the nanofibers are randomly oriented</td>
</tr>
<tr>
<td>alignedstraight.f90</td>
<td>Computes the stiffness matrix of nanocomposite in which the nanofibers are aligned</td>
</tr>
<tr>
<td>interface.f90</td>
<td>Accounts for interface and computes stiffness matrix of inclusion in step-1</td>
</tr>
<tr>
<td>Orienaverage.f90</td>
<td>Accounts for orientation of nanofibers in 2D/3D directions</td>
</tr>
<tr>
<td>ReadNanoCompData.f90</td>
<td>Sends arguments.commands for respective subroutines from the data read by readdata.f90 file</td>
</tr>
</tbody>
</table>
REFERENCES


