EFFECT OF PERFECTLY ALIGNED CNTS
UNDER COHESIVE CRACK BRIDGING IN ADHESIVE JOINTS

by

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ABSTRACT

Recent advances in nano-engineering have prompted the use of nanofillers to strengthen composites and adhesive joints. This is because of the phenomenal mechanical properties that these nanotubes possess. For example, carbon nanotubes have elastic modulus ~1 TPa, and tensile strengths of ~100 GPa, which are more than 300 times those of a polymeric material. It is the purpose of this project to quantify the exceptional effect of nanofillers in cohesive crack bridging in structural adhesive bonds (SABs) for the aircraft industry. In this study, we assume that the high aspect ratio nanotubes are perfectly aligned in a thermoset epoxy adhesive. We carried out finite element modeling of the nano-reinforced SABs taking into account the constitutive law of the nanofillers by using the atomistic-based continuum finite element model. A crack in the nanocomposite is propagated using the virtual crack closure technique and the resulting fracture toughness is calculated. The analysis was conducted using atomic-based continuum finite element in which the constitutive laws for the different phases were carefully selected. Specifically, the Lennard-Jones inter-atomic potentials were used to treat the nanotubes and continuum constitutive laws were used for the SABs. The model represents nanofillers pullout with nonlinear springs and the epoxy is modeled with 2D plane stress elements. Our work reveals that the introduction of perfectly aligned CNTs results in improvements in fracture toughness of the composite of up to 195% at 0.5 wt%. Increasing the weight percentage of carbon nanotube fillers was found to increase the fracture toughness almost linearly. The effect of alignment on the bridging phenomena yields significantly higher toughness values than those typically found experimentally, but this correlates well with studies regarding the effect of nanotube alignment.
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# NOMENCLATURE

- $\delta$: Displacement of the DCB test specimen loading point
- $\sigma$: Maximum tensile strength of a CNT
- $\tau$: Maximum shear strength of a CNT
- $\rho_{\text{CNT}}$: Density of the CNT
- $\rho_{\text{epoxy}}$: Density of the epoxy
- $|\Delta|$: Delamination length correction factor
- $\Delta a$: Crack tip extension length
- $a$: Total cohesive crack length (including the pre-crack length)
- $b$: Width of the DCB test specimen
- $d_{\text{CNT}}$: Diameter of the CNT
- $E$: Young’s modulus of the CNT-reinforced composite material
- $E_{\text{epoxy}}$: Young’s modulus of the neat epoxy
- $E_{\text{plate}}$: Young’s modulus of the carbon plate
- $F_i$: Force normal to the crack propagation plane acting at the crack tip
- $G_{\text{TI}}$: Mode I strain energy release rate calculated at the crack tip
- $G_{\text{CI}}$: Critical mode I strain energy release rate calculated for the composite material
- $K_{\text{IC}}$: Mode I critical stress intensity factor
- $L_{\text{SPEC}}$: Length of the DCB test specimen
- $L_{\text{CNT}}$: Length of the CNT
- $P$: Force at the loading point of the DCB test specimen
- $t_{\text{epoxy}}$: Thickness of the carbon plate for the DCB test specimen
- $t_{\text{plate}}$: Thickness of the carbon plate for the DCB test specimen
- $U$: Total strain energy released as a result of delamination
- $v_l$: Displacement (normal to the crack propagation plane) of the left-adjacent node of the crack tip
- $v_{\text{epoxy}}$: Poisson’s ratio for the epoxy
- $v_{\text{plate}}$: Poisson’s ratio for the carbon plate
- wt%: Percent weight of carbon nanotubes in the epoxy composite
ABBREVIATIONS

APDL  ANSYS parametric design language
ASTM  American Society for Testing and Materials
CFRP  Carbon fibre reinforced polymer
CNT   Carbon nanotube
CSIF  Critical stress intensity factor
COD   Crack opening displacement
DCB   Double cantilever beam
DEM   Displacement extrapolation method
DWCNT Double-walled carbon nanotube
FEM   Finite element method
MWCNT Multi-walled carbon nanotube
RVE   Representative volume element
SAB   Structural adhesive bond
SIF   Stress intensity factor
SEM   Scanning electron microscope
SWCNT Single-walled carbon nanotube
TEM   Transmission electron microscope
VCCT  Virtual crack closure technique
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CHAPTER 1: INTRODUCTION

1.1 STATEMENT OF THE PROBLEM
In the past 30 years, the use of composite materials in aerospace applications has increased dramatically. Composite materials can be designed with superior strength and stiffness while achieving a lower mass than traditional aerospace materials such as aluminum and titanium. With this increased use of composite materials, traditional bonding and joining methods are being replaced. With traditional aerospace materials, joining components through welding and bolting is commonplace. These joining methods are either impossible or often inefficient for use with composite materials. As such, the use of structural adhesive bonds has become more common, leading to new design consideration and potential failure modes.

A popular structural adhesive family used for joining aerospace materials are epoxy polymers. Despite the numerous advantages that epoxy adhesives provide, there are some areas of relative weakness when compared to other joining methods. In particular, the possibility of fracture-based failure of epoxy adhesive joints can be problematic. The relatively low fracture toughness of most aerospace grade epoxies means that fracture is a primary failure method, which can be difficult and expensive to detect. However, the introduction of nano-particle fillers into these epoxies has been found to significantly improve many of the material properties of such adhesives. Nanofillers of all types have been used to toughen plastics [1-4]. For example, experimental results have shown that the fracture toughness of an epoxy can increase by more than 60% over the pure epoxy when only 3.0 wt% of carbon nanotubes are introduced [1]. Other material properties such as tensile strength and stiffness are also improved when CNTs are used [2]. However, in
addition to their beneficial effect on the material properties, carbon nanotubes can also be used as a health monitoring system for the epoxies, whereby the electric resistivity of the adhesive changes if fracture occurs [3; 4]. These modifications allow for significantly more efficient materials, and less costly detection of imminent adhesive failures.

There are still many barriers to overcome before CNT-reinforced epoxies are commonplace; understanding how carbon nanotubes affect the material properties of epoxies being a critical one. While work has been done to develop models of how CNT-reinforcement alters the properties of composites, current models are not complete. Developing a model that can account for the performance increases of the epoxies must account for several of the most important phenomena present in a CNT-reinforced polymer.

It is the purpose of this project to develop a model which will examine the effect that the crack bridging phenomena of carbon nanotube fillers to an epoxy matrix has on the fracture toughness of epoxy adhesives. The model should be used to determine how various epoxy and nanotube parameters affect the fracture toughness. It should be capable of identifying the effect of nanotube length, diameter, and functionalization on the overall performance of the epoxy.

1.2 OBJECTIVES OF THE STUDY
The project scope has been designed to meet the following objectives:

(i) To develop a transient crack propagation model for an epoxy adhesive undergoing DCB loading conditions, capable of estimating the force, displacement, and delamination curves.
To model the crack-bridging phenomena of carbon nanotubes to quantify its effect on the fracture toughness of the adhesive epoxy.

Examine the influence of carbon nanotube concentration on the fracture toughness on CNT-reinforced epoxies through application of the model.

1.3 METHOD OF APPROACH
The model is designed to mimic the ASTM D5528-01 testing standard for determining the fracture toughness of adhesives, commonly known as a double cantilever beam test (DCB). The test layout consists of two carbon plates sandwiching a thin adhesive layer. The test specifications require that the crack is propagated along the neutral axis in the adhesive layer, with an initial crack built into the specimen [5]. A diagram of the test setup is shown in Figure 1-1. This setup is consistent with other efforts to examine crack propagation and extrinsic toughening methods [6; 7]. The model is created using the finite element method, with the ANSYS APDL language used to allow for parameterization. Given symmetry along the crack axis, the model is simplified to account for only one half of the experimental system, where a single carbon plate with a thin adhesive layer is constrained along the symmetry axis and a cantilever style displacement loading is applied at the pre-cracked end of the plate. To model the carbon plate and epoxy adhesive, simple 2D plane elements are used. Using the virtual crack closure technique, the crack is propagated along the constrained neutral axis. To incorporate the carbon nanotube crack bridging, non-linear spring elements are attached to the edge of the adhesive at the symmetry points to simulate nanotubes bridging across the crack plane. The pullout characteristics of the carbon nanotubes from an epoxy matrix are calculated using the atomistic-based continuum model.
By monitoring the force and displacement at the crack tip as well as the crack extension length, and using the calculations derived from elementary beam theory, the stress intensity factor for the composite is calculated. This value is compared to the stress intensity factor of the unreinforced epoxy and the effect of the carbon nanotubes can be assessed. By varying several CNT parameters and properties, such as the carbon nanotube weight percentage, the effects on fracture toughness of adhesive epoxies can be determined.

![DCB Test Specimen](image)

**Figure 1-1: DCB Test Specimen**

### 1.4 LAYOUT OF PROJECT

The report is laid out in five chapters. This introduction forms the first chapter. Chapter 2 provides a literature review of the main concepts utilized in the model: fracture toughness; carbon nanotubes; nano-reinforcement; multi-scale modelling; and crack propagation modeling. Chapter 3 goes into detail about the theoretical model developed for the project, including its implementation, assumptions made, and challenges faced. Chapter 4 contains results and discussion pertaining to the primary areas of study: the effect of weight...
percentage of carbon nanotubes introduced. Finally, a summary of conclusions is contained in Chapter 5.
CHAPTER 2: LITERATURE REVIEW

In order to develop a model for determining the effect of aligned carbon nanotubes on the cohesive fracture toughness of adhesive epoxies, several basic concepts must be explored and understood. This section will review the fundamental background information required, including: a definition of fracture toughness; the basics of carbon nanotubes; the use of CNTs as reinforcing fibres; the current state of understanding on fracture toughness improvements due to CNT-reinforcement, and; the current models used to deal with nano-scale properties.

2.1 FRACTURE TOUGHNESS

Fracture toughness is a concept developed in fracture mechanics, which is defined as the ability of a material with a crack to resist fracture. Linear elastic fracture mechanics states that despite the complex nature of fracture, only a single material property is needed to quantify the resistance to fracture. The fracture toughness, also commonly represented as critical stress intensity factor, is designated by the variable $K_C$. A crack will not grow unless the stress intensity factor at a crack tip is higher than the critical stress intensity factor of the material[8]. Fracture mechanics dictates that there are three different types of fracture that can occur to a body [9]:

I. Opening mode ($K_{IC}$)

II. Sliding mode ($K_{IIc}$)

III. Tearing mode ($K_{IIIc}$)

Fracture is a combination of these modes, and every material has a different propensity to resist these fracture modes.
A closely related concept is strain energy release rate, $G$, which represents the energy available for crack growth [9]. A relatively simple relationship between stress intensity factor and strain energy release rate is available for Mode I fracture (assuming plane stress conditions) [10]:

$$K_{IC} = \sqrt{G/I}$$

There are several types of fracture that can occur in a structural adhesive joint. Two that are particularly important are interfacial and cohesive fracture. Interfacial fracture occurs along the bond surface between the epoxy and one of the bonding materials. Interfacial fracture is dependent on several factors including cohesive fracture toughness, bond surface cleanliness and surface roughness. Cohesive fracture occurs within the adhesive itself (away from the bond surfaces), and is an intrinsic property of the adhesive, unlike interfacial toughness.

There are several ways to measure cohesive fracture toughness, depending on the combination of the three fracture modes desired. For purely opening mode fracture, a common test method consists of loading a double cantilever beam and measuring the applied load, crack extension and cantilever displacement as set out in the ASTM D5528-01 specification[5], and is seen in Figure 1-1. The strain energy release rate calculation used in the standard is based on elemental beam theory, with a derivation provided below [11].

The Mode-I strain energy release rate is defined as:

$$G_I = -\frac{1}{b} \frac{dU}{da}$$

The method of analysing the strain energy release rate is based on a change in compliance of a theoretical test specimen. An example of such a compliance curve is shown in Figure 2-1.
Figure 2-1: Compliance curve of beam specimen

It can be seen that incrementing the displacement by $d\delta$, the total strain energy lost in the system is $dU$: the difference in area of the two graphs. For an infinitesimal increment in crack extension, the strain energy loss in the system can be expressed as follows:

$$-dU = \frac{1}{2} (Pd\delta - \delta dP)$$

Combining these equations provides an equation for solving the strain energy release rate:

$$G_I = \frac{1}{2b} \left( P \frac{d\delta}{da} - \delta \frac{dP}{da} \right)$$
However, most load curves are non-linear and are more difficult to analyse using this method. Hence, data reduction methods have been created. Most commonly, each half of the DCB specimen is considered as a cantilever beam. This assumption yields the following:

$$\delta = B P a^3$$

where B is a property of the test specimen material and geometry. Combining this with the strain energy release rate equation yields the strain energy release rate formula provided in the ASTM standard:

$$G_I = \frac{3P^2Ba^2}{2b}$$

or

$$G_I = \frac{3P\delta}{2ba}$$

### 2.2 CARBON NANOTUBE FUNDAMENTALS

Nano-particles, such as carbon nanotube, are particles that have a critical dimension less than 100 nm. Carbon nanotubes are nano-particles made up of carbon atoms bonded together like a graphite sheet rolled to make a cylinder, and can be formed with a single wall (SWCNT) or multiple walls (MWCNT)[12; 13]. Figure 2-2 shows a schematic of carbon nanotubes on the atomistic-scale.
Carbon nanotubes are of particular interest in the field of nano-reinforcement because they have remarkable mechanical properties. For example, the tensile modulus of a carbon nanotube is 4-5 times greater than that of steel, with a tensile strength as much as 50 times greater than steel, all with close to one-quarter the density of steel [14]. Another important property of carbon nanotubes are their large aspect ratios, which can be significantly higher than those found in micro-particles. A SWCNT can have a diameter significantly less than 2 nm, but can be greater than 18 cm in length [15]. Typically, CNTs with aspect ratios in the hundreds or thousands are considered for composite reinforcement. An image of several MWCNTs is shown in Figure 2-3. It can be seen that the carbon nanotube are not perfect cylinders, but have various kinks and deformations. Also, as a consequence of the
manufacturing methods and the attraction forces between individual nanotubes, CNTs tend to bundle together [16] and form agglomerates[17]. These bundles can be quite large and exhibit properties that are inferior to those of individual nanotubes [16; 17]. While it is possible to align, disperse and distribute nanotubes in polymers using a combination of electric and magnetic fields, or with sonication, mixing and calendering [18; 19], current methods of doing so are not yet satisfactory in this regard.

2.3 CNT-REINFORCED EPOXIES
Introducing carbon nanotubes into epoxies has yielded significant mechanical property improvements. A sample of the literature shows up to 300% increase in the tensile modulus of polypropylene with the introduction of just 1.0 wt% SWCNTs, a 162% increase in tensile strength in Nylon-6 with 2 wt% MWCNTs, and a 140% increase in ductility of polyethylene with 1.0 wt% of MWCNTs [20]. Also, the fracture toughness of the material is significantly
improved, and is discussed in detail in the next section. These mechanical property changes are caused by the remarkable strength and stiffness of the carbon nanotubes, where load is transferred through the epoxy matrix to the nanofillers, similar to the mechanisms occurring in a normal composite material.

To understand how the material transfers these loads, the composite can be broken down into three segments: the filler (carbon nanotubes), the matrix (epoxy) and the interface between the two. While the material properties of the carbon nanotubes and polymer matrix can be determined readily using various theoretical and experimental techniques, the interface between the two is more complex. The interface is formed from interactions between the atoms of the carbon nanotube and those of the polymer interface [21]. These interactions are constructed from several components. The most basic is van der Waals interaction forces from atoms in close proximity to each other. In addition, functionalization of the carbon nanotubes can form covalent bonds between the nanotubes and the polymer matrix. These bonds form at kinks in the carbon nanotube and at their ends, and are used to affect the strength of interface [22; 23]. The pullout properties of CNTs from epoxies are not well understood, and results of experimental testing and simulation do not correlate well. Experimental results yield a pullout that occurs quickly and then dissipates slowly [24; 25], whereas simulations suggest that the pullout force increases more slowly and stays constant almost until full pullout occurs [26]. Given the difficulties in performing experiments in the nano-scale, and the uncertainty inherent in the modeling techniques, it is unknown which results are more reliable.
2.4 FRACTURE TOUGHNESS OF CNT-REINFORCED EPOXIES

Significant research has been done to measure the improvements in fracture toughness that a CNT-reinforced polymer can provide compared to neat epoxies. A summary of some experimental results is provided:

Fieldler et al examine the fracture toughness of CNT/epoxy composites containing functionalized and non-functionalized DWCNT dispersed through shear mixing in an epoxy matrix. The fracture toughness for functionalized DWCNTs was found to increase by as much as 43% compared to the pure epoxy matrix, when a CNT filler content of 0.3 wt% was used. A peak fracture toughness increase of 30% was found for the non-functionalized DWCNTs at the same filler content [18].

Ganguli et al performed single edge notch three-point bending tests on specimens in order to investigate the effects of MWCNTs in a tetra functional epoxy. Samples were prepared using an asymmetric high speed mixer to disperse the filler. Samples of both the neat polymer and a composite containing 1.0 wt% filler content were prepared. Testing of the samples found a 300% increase in the stress intensity factor of the composite sample [27].

Seyhan et al performed experiments to evaluate both functionalized and non-functionalized DWCNTs and MWCNTs in a modified vinyl-ester/polyester hybrid matrix. Using a 3-roll milling process to disperse the CNTs, functionalized CNTs were found to have the most significant increases in fracture toughness. Specifically, the functionalized MWCNTs exhibited a 40% increase in fracture toughness at 0.3 wt% filler content when compared to the neat polymer. Functionalized DWCNTs exhibited a fracture toughness increase of more than 20% at 0.3 wt% nanotube content [28].
Yu et al studied the fracture toughness of MWCNTs/epoxy composites with nanotube contents between 0.0 and 3.0 wt%. Using a sonication dispersion method with a degassing agent to prevent the formation of voids, a maximum increase in toughness of 62-66% at 3 wt% filler content was found over the neat polymer. An increase in fracture toughness of 29-40% at 3 wt% nanotube content was found for samples prepared without the degassing agent [1].

The experimental results have indicated that significant increases in the fracture toughness of the composites were found at even very low filler contents, but toughness reduces as filler content is increased further. The research found that functionalization and dispersion of the CNTs significantly impacted the toughness improvements of the CNTs. More experimental results can be found in Prashantha et al [2], Thostenson and Chou [29], and Zhou et al [30].

2.5 FRACTURE TOUGHNESS MECHANISMS
In order to determine the material properties of many composite materials, the law of mixtures is often used. The law of mixtures states that in order to determine the magnitude of a given property X for a composite C made up of a matrix A (a wt%) with filler B (1-a wt%), you simply ratio the property X of A and B based on the % weights, such that:

\[ X_C = aX_A + (1 - a)X_B \]

However, unlike most composite mechanical properties which can be readily determined using the law of mixtures, this rule cannot explain the fracture toughness improvements of epoxies with CNT fillers. The reason for this is that the fracture of the carbon nanotube rarely occurs, and most of the toughness improvement occurs due to other phenomena [17;
To account for fracture toughness improvements, several mechanisms have been identified in materials that have micro or nano-particles introduced. One of the most prominent mechanisms is an extrinsic toughening mechanism known as crack bridging, where the two ends of a cylindrical particle stay adhered to opposite ends of the crack walls, as the crack propagates [33; 8]. As the crack splits, the fibre is pulled from both walls of the crack and this tension helps prevent the crack from opening further. A diagram of how crack bridging occurs is shown in Figure 2-4.

![Crack Bridging Diagram](image)

**Figure 2-4: Crack bridging phenomena (randomly dispersed fibres)**

The final form of crack bridging is fibre pullout, whereby a fibre spanning the crack is pulled right out of one side of the wall. Because of the large aspect ratios of carbon nanotubes, a third, similar mechanism can also take place. If the interfacial shear strength between the fibre and the epoxy is strong enough and the shear area large enough (typically due to very
long CNTs), fracture of the carbon nanotube can occur instead of pullout [34]. Finally, multi-walled carbon nanotubes can exhibit a sword-in-sheath failure mode whereby one layer of the nanotube fractures, with the other layers still intact. This causes a pullout of the intact tube from a portion of the fractured tube. This failure is similar to normal pullout, as the forces acting on the CNT are van der Waals forces in both cases [26]. This occurs because the bonds holding the CNT ends to the wall are stronger than the CNT layers themselves. Other toughening mechanisms that have been identified on a nano scale are crack pinning and fibre deformation, where the crack direction is changed when coming in contact with a nano-particle and the nanotube deforms due to crack propagation, respectively[18]. These mechanisms have not been shown to significantly contribute to fracture toughness improvement when compared to the effect of crack bridging and fibre pullout.

There has been some work done to experimentally identify nano-scale toughening mechanisms. Xia et al observed crack deflection, crack bridging and fibre pullout in CNT-reinforced ceramic composites through the use of SEM photography [35]. Watts and Hsu used TEM micrographs to identify both CNT bridging and CNT fibre pullout in experiments with MWCNTs [36]. Fielder et al obtained evidence of both DWCNTs and MWCNTs bridging induced cracks in an epoxy using both TEM and SEM [18]. Other evidence of these toughening mechanisms can be found in Prashantha et al [2], W. Zhang et al [37], and Thostenson and Chou [29].

2.6 MODELLING ON THE MACRO AND NANO-SCALES
Another challenge that limits the understanding of nano-particle reinforcement of polymers is the difference in scales between the macro-scaled matrix properties and the nano-sized filler
particles. Carbon nanotubes are made up of only tens of thousands of carbon atoms and cannot be described on the macro-scale. In contrast, our material representations of polymers are based in the macro-scale and are difficult to simulate on the nano-scale. Because of this, different models have approached the problem in a number of ways. Using molecular dynamics, some researchers have attempted to model the polymer matrix and CNT fillers to their individual atoms; however the computing power required to model bonds and forces between each atom at the atomistic scale makes discerning macro-sized properties difficult, as well as allowing limited volumes to be modelled. Others have used hybrid models that have handshaking routines to interact between the macro and nano scales. Another method, the atomistic-based continuum model, uses continuum mechanics at an atomistic scale to model some of the bonds between the atoms in the matrix, which reduces the complexity (and therefore the required computing resources) of the model compared to a molecular dynamics approach, while maintaining a suitable measure of accuracy. The atomistic-based continuum model is discussed in more detail in the next section.

2.7 THE ATOMISTIC-BASED CONTINUUM MODEL

The atomistic-based continuum technique used for this project, developed by Wernik and Meguid at the University of Toronto Engineering Mechanics and Design Lab, uses continuum mechanics to represent atomic structures and inter-atomic interactions. To model carbon nanotubes, a space frame of the nanostructure is modeled using the finite element method. The Modified Morse inter-atomic potential is used to determine the stiffness of elements, which incorporates tensile and angle bending forces. Other bond deformation mechanisms are ignored as they play an insignificant role compared to the forces accounted
for[14]. For the purpose of this research, the atomistic-based continuum model is extended to model nanotube pullout. Most of the epoxy matrix is ignored and the interface between the epoxy and nanotube atoms is represented through the Lennard-Jones inter-atomic potential. Given the number of elements, the size of the nanotubes and surrounding epoxy is small, with only a 5.2 nm CNT being modeled. For more information on the atomistic-based continuum model, refer to Wernick and Meguid [14; 38].

2.8 MODELING CRACK PROPAGATION

Accurately determining the stress intensity factor at the crack tip is needed to transiently propagate a crack in a finite element analysis. Currently, there are several techniques for dealing with stress intensity factor and crack-propagation. Some common methods are the J-integral, Crack Opening Displacement (COD), Displacement Extrapolation Method (DEM), and the virtual crack closure technique (VCCT). Many of these methods rely on using singular elements to develop a stress or energy at the crack tip. However, VCCT can be done with ordinary plane elements and uses the strain energy release rate (GIC) to determine cracking instead of stress. This offers several advantages over other methods, specifically with regards to element size and the ability to use the same mesh at each load step instead of having to remesh in order to incorporate singular elements at the moving crack tip. An example of a typical crack tip modeled for VCCT implementation is shown in Figure 2-5.
The theory behind the virtual crack closure technique is based on the two-step crack closure technique for determining the strain energy release rate at a crack tip. This method assumes that the energy release from a crack extending by length $\Delta \alpha$ is equal to the energy required to close the same crack by length $\Delta \alpha$. The virtual crack closure technique additionally assumes that the force acting on the crack tip is the same as the force required to close the crack a small interval $\Delta \alpha$. Based on these assumptions, the mode I strain energy release rate at the crack tip for the epoxy adhesive can be calculated from the following [10]:

$$ G_{T1} = -\frac{1}{2\Delta \alpha} F_i (v_l - v_{l*}) $$
Similar expressions exist for mode II and mode III strain energy release rates. Note that \( l' \) represents the mirror node of \( l \) on the other side of the crack plane, and \( v_l' \) is equal to \( v_l \) for symmetric problems.

2.9 EXISTING FRACTURE TOUGHNESS MODELS

Several models have been developed to help understand the effects on fracture toughness in CNT-reinforced polymers. Most models attempt to quantify the effects of one particular toughening mechanism using either analytical or numerical methods.

Wichmann et al use an analytic model to capture an upper bound on energy dissipation due to CNT pullout. The problem is approached by scaling the energy dissipation of a microfiber to that of a several carbon nanotubes, relying on volume equivalence to ensure compatibility of parameters. The model assumed tensile strength of carbon fibres and CNTs to be on the order of 1-7 GPa and 30-50 GPa, respectively [39].

Lachman et al uses a pull-out energy dissipation expression to show why an increase in the shear strength of the CNT-epoxy interface improves the fracture toughness of the nano-reinforced composite. They argue that due to the high strength of carbon nanotubes, their critical lengths are often much larger than their typical lengths. This results in pullout being the dominant toughening mechanism, which differs from typical micro-scale fibres where fibre fracture is the primary form of energy dissipation. As a result, an increase in interfacial strength increases the energy absorbed, unlike in micro-scale systems where a decrease in interfacial strength delays fibre fracture [40].
In Blanco et al, a more complex analytic model is created to examine the interlaminar toughness of composite panels that are reinforced with CNT pullout mechanisms, and the results are compared to experimental results. The models for two types of pullout are developed: traditional pullout and sword-in-sheath pullout. The model assumes several parameters for the carbon nanotubes, as well as the polymer matrix. The model indicated that the aspect ratio of the CNTs is critical to the level of fracture toughness improvement. The authors compared the analytic fracture toughness improvements to those of experimentation, and found poor correlation between results, with experimental values falling between the traditional pullout and sword-in-sheath results. This was attributed to the pullout being a combination of sword-in-sheath pullout and fibre pullout, as well the presence of other toughening mechanisms that were not considered in the model, agglomeration of CNTs, and other experimental conditions [34].

Seshadri and Saigal develop an analytical model for CNT crack bridging of viscoelastic polymers in an attempt to identify the parameters associated with the improvements in fracture toughness. The authors derive expressions for elastic and viscoelastic polymer pullout stiffness, as well as fracture energy augmented by a single nanotube bridge. The model assumes that CNT pullout is the idealized case of crack bridging, one nanotube pullout does not affect other nanotubes (high dispersion and low volume fraction) and that the nanotubes are rigid bodies (infinitely stiff). The authors validate their analytic model of pullout stiffness using a numerical simulation, and find good correlation in results between the two methods (but do not attempt to correlate results with experimental data). They conclude that augmented fracture energy is dependent on several
parameters, including crack opening rate, interface stiffness, nanotube density, and viscoelastic relaxation of the polymer [41].

W. Zhang et al use an analytic model to predict the crack propagation rate of SWCNT and MWCNTs in an epoxy resin, as a function of stress intensity factor. They consider fibre pullout the primary source of toughening and assume that a constant force is required throughout the pullout. They also generate an expression for the crack bridging length. From this, the pullout work for each nanotube is calculated and incorporated into a new stress intensity factor, which also incorporates the number density and fibre orientation of the nanotubes. They use experimental data to calibrate and validate their model, where good correlation is found. The model finds that the crack propagation rate decreases as the weight fraction of CNTs is increased. The model also shows that as stress intensity increases, the suppression of crack growth rate for the nanotube composites degrades, when compared to the neat epoxies [37].

Shi et al use a hybrid atomistic/continuum model to examine the fracture of zigzag and armchair CNTs in a polymer matrix, which helps to indentify the parameters which affect defect formation, as well as the effect of the polymer matrix on the critical breaking strain of the CNT. The authors assume that the CNTs are straight fibres, there is no residual strain in the composite and that the CNT-matrix interface is perfectly bonded. The model found that a stiffer polymer matrix reduced the fracture strain of the CNT, implying that CNTs are less effective at releasing energy when in a polymer matrix, as opposed to when they are not imbedded in a composite. The model looks only at CNT fracture as an energy dissipation method [42].
CHAPTER 3: ATOMISTIC-BASED CONTINUUM MODEL OF CRACK BRIDGING IN SABs

3.1 OVERVIEW

The finite element model, created in the ANSYS APDL language, is a non-linear transient system which iteratively propagates a crack. The model is simplified to two dimensions (2D) and mimics a double cantilever beam test. Furthermore, since there is symmetry between the two sides of the beam, only one half of the system is modelled. In total, the model consists of a carbon plate, an epoxy adhesive, carbon nanotubes and ultra-stiff symmetry elements.

There are two primary phases of the model:

1. Pre-crack cantilever extension phase
2. Crack propagation phase

During the pre-crack cantilever extension phase, an incremental displacement is applied to the cantilever (point A as shown in Figure 3-1), and the beam bends similarly to a simple cantilever beam. After each iteration in the pre-crack phase, the stress intensity factor at the crack tip is calculated to determine whether crack-propagation should begin.

Figure 3-1: DCB Model under loading
Once the stress intensity factor at the crack tip exceeds the critical stress intensity factor of the adhesive, the model enters the crack propagation phase.

During the crack propagation phase, the stress intensity factor of the crack tip is calculated much the same way as in the pre-crack phase. However, when the SIF at the crack tip is higher than the critical value, the crack tip element constraint is broken, thereby extending the crack tip as seen in Figure 3-2.

Figure 3-2: Crack tip propagation (a) SIF below critical; (b) SIF at critical value; (c) Crack tip extended
During this second phase, the crack tip will have extended to where carbon nanotubes will be spanning across the crack, thereby pulling out and contributing to the strain energy absorbed by the material. This pullout force is derived from inter-atomic forces acting in the interface between the carbon nanotube and the epoxy, and is represented by non-linear springs. Once the crack extends to beyond the CNT length, the element no longer contributes a force, as the CNT has been completely pulled out from the system.

3.2 MATERIAL PROPERTIES AND SPECIMEN PARAMETERS

In order to generate simulation results that are very close to experimental data, material property data was based on the expected values of materials selected for experimental validation. The properties of the carbon nanotubes are assumed based on data from the atomistic based continuum model.

<table>
<thead>
<tr>
<th>Material and specimen properties</th>
<th>Carbon Plate</th>
<th></th>
<th>Epoxy Adhesive</th>
<th>Carbon Nanotube</th>
<th>Specimen Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Young's Modulus (E&lt;sub&gt;plate&lt;/sub&gt;)</strong></td>
<td>100.00 GPa</td>
<td><strong>Young's Modulus (E&lt;sub&gt;epoxy&lt;/sub&gt;)</strong></td>
<td>3.43 GPa</td>
<td><strong>Length (L&lt;sub&gt;CNT&lt;/sub&gt;)</strong></td>
<td>1000.00 nm</td>
</tr>
<tr>
<td><strong>Poisson's Ratio (ν&lt;sub&gt;plate&lt;/sub&gt;)</strong></td>
<td>0.30</td>
<td><strong>Poisson's Ratio (ν&lt;sub&gt;epoxy&lt;/sub&gt;)</strong></td>
<td>0.30</td>
<td><strong>Diameter (d&lt;sub&gt;CNT&lt;/sub&gt;)</strong></td>
<td>10.00 nm</td>
</tr>
<tr>
<td><strong>Density (ρ&lt;sub&gt;epoxy&lt;/sub&gt;)</strong></td>
<td>4.80 kg/m³</td>
<td><strong>Max. Stress Intensity (K&lt;sub&gt;Ic&lt;/sub&gt;)</strong></td>
<td>0.650 MPa√m</td>
<td><strong>Density of CNTs (ρ&lt;sub&gt;CNT&lt;/sub&gt;)</strong></td>
<td>1.35 kg/m³</td>
</tr>
<tr>
<td><strong>Length (L&lt;sub&gt;SPEC&lt;/sub&gt;)</strong></td>
<td>127.00 mm</td>
<td><strong>Width (b)</strong></td>
<td>25.40 mm</td>
<td><strong>Thickness of Carbon Plate (t&lt;sub&gt;plate&lt;/sub&gt;)</strong></td>
<td>4.00 mm</td>
</tr>
<tr>
<td><strong>Thickness of Epoxy Adhesive (t&lt;sub&gt;epoxy&lt;/sub&gt;)</strong></td>
<td>0.20 mm</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3-1: General material and specimen properties used in the finite element model
3.3 CRACK-BRIDGING MODEL ASSUMPTIONS

3.3.1 Alignment, dispersion and distribution of the carbon nanotubes

Implementing the carbon nanotube pullout into the model is a significant challenge. Due to limited computer power and resources, the model cannot be made fine enough to account for individual nanotubes. In addition to this problem, carbon nanotubes are not the simple, straight pipes they are being represented as. They can be curved, wrap around each other and are never evenly aligned, dispersed and distributed throughout an epoxy mixture, despite all efforts to make them that way [18]. An image of a small carbon nanotube agglomerate dispersed in an epoxy is given in Figure 3-3. As such, significant assumptions need to be made about the properties of the nanotubes. In particular, it is assumed that all nanotubes are aligned normal to the crack plane, and are equally dispersed and distributed across the symmetry line.

Given the material properties of the carbon nanotubes and the epoxy shown in Section 3.2, a formula can be derived for the number of carbon nanotubes that will be present in a given volume of epoxy, with respect to the weight percentage of nanotubes. In order to incorporate the assumptions about the alignment, distribution and dispersion of the CNTs in our model, a system is defined with a single CNT encompassed by epoxy, as shown in Figure 3-4.
Figure 3-3: Carbon nanotubes in an epoxy matrix
The height of the rectangle is chosen to be the same as the length of the carbon nanotube, and the length and width (both $d$) is to be calculated such that the rectangle contains the desired wt% of CNT. The formula to describe the composite such that it satisfied all the specimen parameters is as follows:

$$d = \sqrt{\frac{V_{CNT} \cdot \rho_{CNT}}{L_{CNT} \cdot \rho_{epoxy} \cdot \text{wt} \%}} - \frac{V_{CNT}(\rho_{CNT} - \rho_{epoxy})}{L_{CNT} \cdot \rho_{E}}$$

Given that the carbon nanotubes need only be modeled around the crack propagation zone, the total epoxy volume of interest is the area of the bonded epoxy in the crack plane, times the height of a carbon nanotube. From this, the total number of CNTs along the crack plane is calculated by dividing the total cohesive volume ($L_{SPEC} \times b \times L_{CNT}$) by the volume of our
rectangle \((d^2 \times L_{\text{CNT}})\). As described in the implementation section (3.4.5), multiple CNTs are combined into a single non-linear spring element, based on the distance between nodes and the thickness of the specimen.

It is apparent that this assumption overestimates the contribution of carbon nanotubes. In reality, most carbon nanotubes would not be perfectly aligned, and many nanotubes would be unevenly dispersed, or even wrapped together to form large agglomerations that do not exhibit ideal fibre pullout behaviour. However, quantifying these factors is virtually impossible and not required given that the expected simulation results are to be used as an upper bound on the crack-bridging potential of the carbon nanotubes.

3.3.2 Crack bridging vs. nanotube pullout

For the purposes of modeling, crack bridging is essentially considered an incomplete form of nanotube pullout. It is also assumed that the CNTs are not so long that CNT fracture occurs. This assumption is made in other theoretical models, and can be validated by comparing the maximum pullout force of the carbon nanotube from the epoxy to the tensile force required to fracture the carbon nanotube. This is done using the critical length formula, and is shown below [40]:

\[
L_{\text{CNT}} = \frac{\sigma r_{\text{CNT}}}{\tau}
\]

Using a tensile strength of 114.4 GPa [14], a shear strength of 30 MPa [40] and a radius of 5 nm (based on the assumed CNT in this project), it can be seen that the longest CNT for which this assumption is valid is 19.0 \(\mu\)m long, which is much longer than the length considered in the model (1.00 \(\mu\)m).
Also, it is assumed that all the CNTs are single-walled, thereby eliminating a possible sword-in-sheath pullout mode, which might occur with MWCNTs.

3.3.3 Interfacial shear strength

The constitutive law for the carbon nanotube elements was designed based on the results of a pullout simulation using the atomistic-based continuum model. Given the huge number of elements involved in the simulation, the longest CNT modeled using the atomistic-based continuum model was only 5.2 nm long, which is much less than the size of the CNTs used for epoxy reinforcement. In order to account for this difference, the profile generated for nanotube pullout was determined using the atomistic-based continuum model, and the peak force of the profile was determined based on a shear strength of 30 MPa, which is a commonly cited figure [40].

In addition to this method of calculating the constitutive law of the CNT pullout elements, another critical assumption about the bonds has been made. The only types of forces acting between atoms are through Lennard-Jones potentials, and the carbon nanotubes are not functionalized. If the CNTs were at all functionalized, there could be even higher pullout forces, leading to further increases in fracture toughness’s and a greater potential for CNT fracture [21]. If functionalization of the CNTs was desired, the constitutive law of the pullout would change drastically and covalent bonds would need to be modeled in the atomistic-based continuum model to generate this new law.
3.3.4 Effect of CNTs on epoxy material properties

It is assumed that the introduction of the carbon nanotube fillers into the epoxy matrix has no effect on the mechanical properties of the epoxy matrix, other than the crack bridging phenomena represented by the nonlinear springs. This is obviously not valid, as the total volume of epoxy is going down, and the epoxy is no longer a homogenous substance and there are several other mechanisms that play a role in the toughness of the composite. However, the other effects of CNTs in the matrix itself are the subject of separate research. Should these effects be known, they can be incorporated to account for this discrepancy.

3.4 F.E.M IMPLEMENTATION

3.4.1 Modeling the epoxy and carbon plate

Both the epoxy adhesive and the carbon plate are modeled using PLANE182 elements assuming plane stress with a specified thickness. Because the crack is forced to propagate along the neutral axis (which is far from the adhesive/plate interface), the shear stresses that occur along the interface are not significant to the problem. The material and specimen properties used for these elements are described in Table 3-1 (see page 25). An image showing the layout of elements is provided in Figure 3-5.
3.4.2 Applying the symmetry constraints

In order to implement symmetry constraints along the neutral axis that can be easily disabled to propagate the crack, rigid interface elements must be introduced that connect the nodes of the 2D plane elements of the epoxy to constrained nodes [43]. To do this, COMBIN14 elements with a very high stiffness are used. These elements are used because they can be disabled during load stepping and their nodes are designed to be coincident.

3.4.3 Application of the virtual crack closure technique

The virtual crack closure technique is used to calculate the stress intensity factor at the crack tip. Because the DCB test is symmetric along the crack propagation axis, the strain energy release rate formula can be modified. By applying the symmetry conditions, calculation is simplified to:
\[ G_{TI} = -\frac{1}{\Delta a} F_i v_l \]

Therefore the stress intensity factor of the epoxy at the crack tip is equal to:

\[ K = \sqrt{G_{TI} E} = \sqrt{-\frac{E}{\Delta a} F_i v_l} \]

In order to propagate the crack, the location of the crack tip is monitored and the stress intensity factor of the epoxy is calculated after each load step. If the VCCT calculated stress intensity factor exceeds the critical stress intensity factor of the neat epoxy adhesive (which is based on experimental results from Fielder et al [18]), the rigid symmetry element constraining the epoxy at the crack tip is disabled, extending the crack along the neutral axis.  

Because of the discrete nature of the virtual crack closure technique, whereby individual elements are disabled to allow the crack to propagate, important consideration has to be taken with respect to both the element size and the load point displacement increment per load step. If the incremental deflection of the cantilever beam is too high and the element length (along the crack propagation axis) too small, the crack will not be able to propagate fast enough and the VCCT fracture toughness will exceed the allowable value. Alternatively, if the element length is too large and the beam separates very little per increment, a single crack increment could reduce the VCCT fracture toughness so much that several load steps are required to get it back to the limit value. A figure demonstrating the issues that an improper load step size can cause is shown in Figure 3-6.
The model requires that the VCCT measured fracture toughness be as close to the critical fracture toughness of the epoxy as possible for the entire duration of the crack propagation event. While this is difficult to achieve in practice, keeping the value as stable as possible can significantly improve the accuracy of the model. To ensure this, the load step size is adjusted after each step to bring it closer to the optimal value. This is done by calculating the difference between the previous fracture toughness and the current fracture toughness. This difference proportionally increases or decreases the step size if undershoot or overshoot occurs, respectively.

Figure 3-6: Effect of improper load step on solution
3.4.4 Modeling the carbon nanotubes

The carbon nanotube elements introduced in the model are designed to simulate full nanotube pullout, and are not meant to represent the properties of the CNTs themselves. Modeling of the carbon nanotube pullout is done with COMBIN39 elements. There were two pullout models generated: one based on a computer model, and another based on experimental results. For the first pullout element, the stiffness follows a non-linear shape, which is based on the pullout profile generated by the atomistic-based continuum model for CNT-pullout with a peak force determined from commonly cited shear strengths. The second pullout element is designed to mimic that of experimental results, with a peak force based on commonly cited shear strengths. The constitutive profiles of both elements (single CNT) are shown in Figure 3-7. The force-displacement curve goes to zero after the pullout distance exceeds the length of the CNT so that it has no further impact on the model. For the most part, the pullout profile used to gather results is based on the atomistic-based continuum model. This is because there are very few experimental results and they are not as reliable. However, convergence testing was done with the experimental-based profile, because such a profile requires smaller element sizes to capture the effects of crack-bridging.
Because of the scaling difficulties and the number of epoxy elements required to account for individual carbon nanotubes in the mesh, the system has been simplified by combining several CNTs dispersed along the surface of the crack wall into a single CNT, thus reducing the total number of elements. This is also required to reduce the system to 2D from 3D (see Figure 3-8).

Figure 3-7: Constitutive laws of CNT pullout from epoxy (simulation and experimental-based elements)

Figure 3-8: Simplification of nanotube elements
3.4.5 Calculating the composite critical stress intensity factor

To calculate the composite stress intensity factor (which represents the improved fracture toughness of the nano-reinforced composite), the beam theory method specified in the ASTM standard is used. Where \( P \) is the load at the application point, \( \delta \) is the load point displacement, \( b \) is the specimen width and \( a \) is the delamination length, the strain energy release rate of a double cantilever beam is:

\[
G_{CI} = \frac{3P\delta}{2ba}
\]

The strain energy release rate is then converted to critical stress intensity factor \( K_{IC} \) through the following formula:

\[
K = \sqrt{G_{CI}E}
\]

3.5 CONVERGENCE AND MODEL OPTIMIZATION

Balancing solution time and accuracy requires the selection of a suitable crack increment, \( \Delta a \), which is directly dependant on element size. If the crack growth increment is too large, the number of elements in the crack bridging zone will be too small to properly model the effect of carbon nanotubes. If the increment is too small, the solution time is unnecessarily long, and computer resources may not be adequate to solve the system. In order to optimize the selection, simulations were run with a number of growth increments and the stress intensity factors were compared. The simulations were run with 0.25 wt% carbon nanotubes and the pullout profile was based on experimental results. This profile was selected because the experimental pullout profile has a very small force peak compared to the simulation results,
requiring a smaller crack growth increment for the same nanotube length. Figure 3-9 shows the results converging to a solution.

![Figure 3-9: Effect of crack growth increment on solution convergence](image)

It can be seen that at large crack increments, there is only a small impact on fracture toughness. This is because there are too few intervals in the crack bridging zone to allow for the full impact of the CNT pullout profile. When the interval gets to be smaller (highlighted section), we can see that the toughness plateaus again, and the full effect of the bridging is being seen. Therefore, the optimal increment for crack growth per load step was selected to be 7.8125 μm, which corresponds to 128 elements/mm.
A difficulty encountered with the model in solving systems with a high concentration of CNTs was that the number of pullout elements in the crack propagation zone were too small, with each pullout element significantly contributing to the fracture toughness. This creates significant convergence issues as there is a very sharp drop off once the nanotube pullout occurs. In order to resolve this issue, a finer mesh would be required around the crack bridging zone, which would allow for more pullout element which individually contribute less to the toughness. Because of the computing power required to implement this, high concentrations of CNTs (>0.50%) were not able to be tested with the model.
CHAPTER 4: THEORETICAL RESULTS AND DISCUSSION

4.1 ANALYSIS OF THE NEAT EPOXY

The first analysis done with the newly constructed model is to validate the accuracy of the model in known conditions; namely with the neat epoxy. With the parameters set out in Table 3-1 for the specimen and epoxy, a test was run to ensure that the composite critical stress intensity factor (calculated from specimen results as in Section 3.4.5) matched the critical stress intensity factor of the epoxy (calculated at the crack tip as per Section 3.4.3). A sample of the calculations and results is provided below.

After the analysis is completed, a load-crosshair displacement curve is generated, as shown in Figure 4-1.

Figure 4-1: Load-displacement curve of DCB loading of neat epoxy
From this curve and the data gathered regarding delamination length, the following calculations are made based on the ASTM D5528-01 standard, discussed in Section 3.4.5.

<table>
<thead>
<tr>
<th>Neat epoxy data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Load</td>
<td>80.278</td>
</tr>
<tr>
<td>Displacement @ Peak Load</td>
<td>0.700</td>
</tr>
<tr>
<td>Peak Delamination</td>
<td>50.241</td>
</tr>
<tr>
<td>Offset Displacement</td>
<td>0.714</td>
</tr>
<tr>
<td>Offset Load</td>
<td>77.520</td>
</tr>
<tr>
<td>Offset Delamination</td>
<td>51.171</td>
</tr>
<tr>
<td>Composite $K_{IC}$ (peak)</td>
<td>0.6733</td>
</tr>
<tr>
<td>Composite $K_{IC}$ (offset)</td>
<td>0.6621</td>
</tr>
</tbody>
</table>

Table 4-1: Neat epoxy fracture toughness calculations

It can be seen that the fracture toughness, 0.6621 MPa√m, is within 1.85% of the specified fracture toughness of 0.650 MPa√m.

4.2 ANALYSIS OF CNT-REINFORCED EPOXIES

4.2.1 Effect of varying concentration of CNTs (wt%)

The most basic analysis of CNT-reinforced epoxies studies the effect of increasing the number of CNTs in the composite. Using the calculation method from Section 3.3.1, the number of nanotubes bridging along the interface is calculated and summarized for multiple weight percentages in Table 4-2.

<table>
<thead>
<tr>
<th>Weight Percentage</th>
<th>Length of Enclosing Square [nm]</th>
<th>Total Number of CNTs</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05%</td>
<td>210.32</td>
<td>43,754,396,920</td>
</tr>
<tr>
<td>0.10%</td>
<td>148.81</td>
<td>87,397,262,074</td>
</tr>
<tr>
<td>0.25%</td>
<td>94.30</td>
<td>217,660,915,179</td>
</tr>
<tr>
<td>0.50%</td>
<td>66.89</td>
<td>432,575,697,035</td>
</tr>
</tbody>
</table>

*NOTE: CNT diameter = 10nm, length = 1.0 um

Table 4-2: Total CNTs bridging the interface at specified concentrations
Simulations for each of the cases were run and the composite critical stress intensity factor was calculated for each case. A plot of fracture toughness with respect to CNT weight percentage is provided in Figure 4-2.

Figure 4-2: Effect of CNT concentration of fracture toughness
Table 3-1 summarizes the results.

<table>
<thead>
<tr>
<th>Weight Percentage</th>
<th>Peak $K_c$ [MPa$\sqrt{m}$]</th>
<th>Change in toughness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00%</td>
<td>0.650</td>
<td>0.00%</td>
</tr>
<tr>
<td>0.05%</td>
<td>0.745</td>
<td>14.62%</td>
</tr>
<tr>
<td>0.10%</td>
<td>0.800</td>
<td>23.08%</td>
</tr>
<tr>
<td>0.25%</td>
<td>1.283</td>
<td>97.38%</td>
</tr>
<tr>
<td>0.50%</td>
<td>1.871</td>
<td>187.85%</td>
</tr>
</tbody>
</table>

Table 4-3: DCB simulation results

4.3 DISCUSSION OF RESULTS

When comparing the specified toughness of the neat epoxy to the calculated results of the simulated neat epoxy, we get very good correlation. This baseline test validates the premise of the model and the implementation of the virtual crack closure technique. The discrepancies can be largely attributed to basic VCCT assumptions and slight oscillation of the solution caused by the discrete nature of the model. Reducing the element sizes may result in even more accurate values, but the current accuracy of the model is acceptable in this regard.

In examining the nano-reinforced composite, the model shows that the introduction of CNTs in an epoxy matrix significantly affects the fracture toughness of the composite. With small concentrations of carbon nanotubes (0-0.1 wt%), the results of both the model and experiments follow the same trend and yield close to expected results, though perhaps slightly higher. However, experiments have found that the fracture toughness of CNT-based nanocomposites decreases when the concentration of crosses a threshold (>2 wt%). This phenomenon could not have been accounted for in the current model. The increase in
fracture toughness was expected to be perfectly linear with the increase in concentration, which was not the case. This is explained by the discretized nature of the pullout elements, of which there were very few acting at a time. As such, the most correct solution would have a CNT pulling out at the peak locally measured fracture toughness, which did not always happen. This may have resulted in some values of fracture toughness to be underestimated (see discussion in Section 3.5).

At 0.1 wt%, the fracture toughness calculated by the model is 23.0% higher than that of the neat epoxy, which is similar to results found in a number of sources (see section 2.4). Beyond this, the fracture toughness increases much higher than typically seen in experimental results. There are several important factors that have been found to play a role in these differences. The alignment of CNTs has been found to significantly affect the fracture toughness of nanocomposites, where perfectly aligned nanofillers can have 5 times the effect as compared to the randomly aligned case [44; 45]. Also, the effect that perfect dispersion has on nanocomposites has not been experimentally determined, but poor dispersion leading to large agglomerations is considered to be the most significant cause of poor nanocomposite performance [17]. As such, it is expected that the fracture toughness calculations should be significantly higher than experimental results from the literature.

In fact, the fracture toughness at 0.1 wt% is lower than would be expected, given that it is comparable to some experimental results. From this and the differences apparent at higher concentrations, it is apparent that other toughening mechanisms also play a significant role in the fracture toughness.
CHAPTER 5: CONCLUSIONS

5.1 SUMMARY

The use of carbon nanotubes as reinforcing agents for epoxy adhesive joints provides considerable improvements in the mechanical properties of such bonds. The current understanding of the mechanisms that provide these improvements is still in its infancy. This report summarizes work done to understand and quantify the effect that the crack bridging mechanism has on the fracture toughness of epoxy adhesives. A finite element model was created that was capable of determining the fracture toughness improvements that introducing CNTs has on an epoxy. The effect of weight percentage of CNTs was simulated.

From the results of the simulations, the following conclusions have been made:

(i) Carbon nanotube crack-bridging increases the fracture toughness of epoxy adhesives.

(ii) As the concentration of CNTs in the adhesive is increased, the rate of toughness improvements decreases

(iii) Mechanisms not directly related to crack bridging (including agglomeration) are responsible for the poor toughness properties of epoxies with high concentrations of CNTs

5.2 FUTURE WORK

There is room for significant improvement with the model, which was not able to be completed due to time restrictions. The first area of work to be done is extending the scope of the project to examine the length and diameter effects of the carbon nanotubes. This
would require different pullout profiles for each carbon nanotube to be generated and several more tests to be run.

The second area of work would be in increasing the accuracy of the model. Optimizations could be done in several of the algorithms to improve to speed of the solution, thereby allowing smaller element increments in a reasonable time. Additionally, the model could be modified to allow for a very fine mesh only in the area of crack growth, instead of along the entire symmetry plane. This would reduce the number of elements without significant impact on the accuracy of the solution. Reducing the size of the DCB specimen would also reduce the number of element and allow for better resolution of the bridging CNTs, if certain parameters were maintained [46]. To further ensure the model is accurate, a convergence check of the joint stiffness could be performed to verify the effect of joint stiffness on model convergence and to ensure an appropriate value was selected.

The third major area of future work on the model is in regards to the properties that the model takes into account for its solution. In particular, introducing other effects of carbon nanotubes on the epoxy would yield a significantly more accurate solution. In particular, some way of accounting for the changes in other material properties of the CNTs such as the tensile modulus of elasticity would improve the model. Also, accounting for the CNTs in this way may shed some additional light on why the fracture toughness decreases at high wt% concentrations. Finally, the model could also be improved to account for randomly dispersed CNTs, account for functionalization of CNTs, and for CNT fracture.
REFERENCES


APPENDIX A: ANSYS APDL SOURCE CODE

! ANSYS DCB Test Model
! Ben Cornwell-Mott
! August 19th 2010
!

! -Comment on Units-
! Length = millimeters
! Force = newtons
! Mass = megagrams

! -START OF CODE-

/CONFIG,NRES,50000

/ PREP7

! Define Parameters (STUFF TO CHANGE)

*SET,CNT_diam,1.000e-5  ! Full diameter of the CNT
*SET,CNT_length,1.000e-3  ! Full length of the CNT (not half length)
*SET,CNT_dx,1e-6  ! Distance between CNTs
*SET,CNT_length_divs,1600973.60  ! Number of CNTs that need to be across the length (in one row)
*SET,CNT_layers,533657.8652  ! Number of rows of CNTs

*SET,SPEC_length,125.0  ! Length of the test specimen
*SET,SPEC_height,0.1  ! Thickness of the test specimen
*SET,SPEC_thick,25.4  ! Width of the test specimen
*SET,SPEC_divs,1400  ! Number of divisions in the specimen
*SET,SPEC_HPd,10  ! Number of divisions in the specimen

*SET,TEST_yinc,150e-4  ! Incremental movement of crosshair
*SET,TEST_tinc,0.150  ! Incremental increase in time
*SET,TEST_yincs,5e-4  ! Incremental movement of crosshair (when crack is propagating) (5.35e-4)for800divs
*SET,TEST_tincs,0.005  ! Incremental increase in time (when crack is propagating)
*SET,SPEC_wtp,1.00

*SET,CP_height,2.85  ! Define the material modulus of elasticity
*SET,CP_moe,1.00e5
*SET,CP_PRxy,0.3  ! Define the material poisson's ratio
*SET,CP_dens,5.800e-9  ! Define the material density
! Define the modulus of elasticity of the rigid joint
*SET,JOMT_moe,1e10

! Initial movement of crosshair
*SET,TEST_yinit,2.85e-1

! Initial increase in time
*SET,TEST_tinit,0.285

! Define the material modulus of elasticity
*SET,RVE_moe,3.43e3

! Define the material poisson's ratio
*SET,RVE_PRxy,0.3

! Define the material density
*SET,RVE_dens,4.800e-9

! Define the material equivalent stress
*SET,RVE_MAX_EQV,3e-5

! Length of the pre-crack
*SET,STARTD,50.0

! Maximum number of load steps
*SET,MAX_COUNT,1000

! Temporary variables
*SET,tempx,0
*SET,tempy,0

! Tracking information for displacement and time
*SET,T_TIME,TEST_tinit
*SET,T_DISPY,0

! More temp variables (STUFF NOT TO CHANGE)

*SET,grid_x,0.0001
*SET,grid_y,0.0001

! - START BUILDING THE MODEL -

/PREP7
N,1,2*SPEC_length

! Set the coordinate system to cartesian
csys,0

! Calculate the element size based on the CNT length
!(so that there are 4 elements between the end of the CNT and the midsection)
grid_x = SPEC_length / (SPEC_divs*SPEC_HPĐ)
grid_y = (2*grid_x)

*SET,SPEC_numdof,(SPEC_length/grid_x)
*SET,SPEC_cntdof,((SPEC_length-STARTD)/grid_x) !number of dofs
within the bonded area
*SET,CNT_proxys,(CNT_length_divs/SPEC_cntdof) !number of CNTs that
occur within one grid point (one row)
*SET,START,NINT(STARTD/grid_x) !number of intervals
between loading point and crack tip

! Define the polymer element
ET,1,PLANE182
KEYOPT,1,1,0
KEYOPT,1,3,3
KEYOPT,1,6,0
KEYOPT,1,10,0
R,1,SPEC_thick,
MPTEMP,,,,,,,,
MPTEMP,1,0
MPDATA,EX,1,,RVE_moe
MPDATA,PRXY,1,,RVE_PRxy
MPDATA,DENS,1,,RVE_dens

! Define the CNT rod (nonlinear)
ET,5,COMBIN39
!* KEYOPT,5,1,0
KEYOPT,5,2,1
!KEYOPT,5,3,2
KEYOPT,5,4,3
KEYOPT,5,6,0

! Non-linear profile of the CNT pullout (using a peak force of 942 nN)
R,5,0,0,0.1*CNT_length,CNT_proxys*CNT_layers*9.42e-7*0.8,0.25*CNT_length,CNT_proxys*CNT_layers*9.42e-7,
RMORE,0.85*CNT_length,CNT_proxys*CNT_layers*9.42e-7,0.90*CNT_length,CNT_proxys*CNT_layers*9.42e-7*0.75,CNT_length,1e-11,
RMORE,CNT_length*1.05,1e-11
MPTEMP,,,,,,,,
MPTEMP,1,0
MPDATA,DAMP,5,,0

! Define the carbon plate element
ET,4,PLANE182
KEYOPT,4,1,0
KEYOPT,4,3,3
KEYOPT,4,6,0
KEYOPT,4,10,0
R,4,SPEC_thick,
MPTEMP,,,,,,,,
MPTEMP,1,0
MPDATA,EX,4,,CF_moe
MPDATA,PRXY,4,,CF_PRxy
MPDATA,DENS,4,,CF_dens

! ------------------------ DEFINE THE POLYMER ------------------------

MAT,1
TYPE,1
REAL,1
ESYS,0

! Define the boundary KPs
K,1,0,0,0
K,2,0,SPEC_height,0
K,3,0,SPEC_height,0

*DO,DI_1,4,5+ 3*(SPEC_divs-1),3
   tempx = tempx + SPEC_length/SPEC_divs
   K,DI_1,tempx ,0,0
   DI_1 = DI_1 + 1
   K,DI_1,tempx ,SPEC_height,0
   DI_1 = DI_1 + 1
   K,DI_1,tempx ,SPEC_height,0
*ENDDO

! Create lines between the keypoints
L,1,2 !Line 1
*DO,DI_1,1,1 + 3*(SPEC_divs-1),3
   !Horizontal Lines
   L,DI_1,DI_1+3
   L,DI_1+1,DI_1+4
   !Vertical Lines
   L,DI_1+3,DI_1+4
*ENDDO

! Create the areas
*DO,DI_1,1,3*(SPEC_divs),3
   AL,DI_1,DI_1+1,DI_1+3,DI_1+2 !Fine mesh area
*ENDDO

! Assign parameters to currently defined areas
AATT,1,1,1,0

MSHKEY,1
MSHAPE,0,2D

*GET, NUM_LINES, LINE, 0, COUNT

! ------------------------- DEFINE THE RIGID CARBON SHEET -------------------------

MAT, 4
TYPE, 4
REAL, 4
ESYS, 0

tempx = 0
! Define the boundary KPs
K, 1000001, 0, SPEC_height, 0
K, 1000002, 0, SPEC_height + CF_height, 0
K, 1000003, 0, SPEC_height + CF_height, 0

*DO, DI_1, 4, 5 + 3*(SPEC_divs - 1), 3
  tempx = tempx + SPEC_length/SPEC_divs
  K, 1000000 + DI_1, tempx, SPEC_HEIGHT, 0

  DI_1 = DI_1 + 1
  K, 1000000 + DI_1, tempx, SPEC_height + CF_height, 0

  DI_1 = DI_1 + 1
  K, 1000000 + DI_1, tempx, SPEC_height + CF_height, 0

*ENDDO

L, 2, 1000002 !Line 1
*DO, DI_1, 1, 1 + 3*(SPEC_divs - 1), 3

  !Horizontal Lines
  L, DI_1, DI_1 + 4
  L, 1000000 + DI_1 + 1, 1000000 + DI_1 + 4

  !Vertical Lines
  L, DI_1 + 4, 1000000 + DI_1 + 4

*ENDDO

! Create the areas
*DO, DI_1, 1, 3*(SPEC_divs), 3
! Define the sizing constraints of the two zones
ESIZE, grid_x*18
LESIZE, 1, grid_y
*DO, DI_1, 2, 1+3*SPEC_divs, 3
  ! Horizontal Lines
  LESIZE, DI_1, grid_x
  LESIZE, DI_1+1, grid_x
  LESIZE, NUM_LINES+DI_1+1, grid_x
  ! Vertical Lines
  LESIZE, DI_1+2, grid_y
*ENDDO

! Set the meshing parameters

MSHKEY, 1
MSHAPE, 0, 2D

! Mesh the solid
AMESH, ALL

! ------------------- DEFINE INITIAL BCs -------------------
! Set the initial symmetry conditions
*DO, DI_1, 1, SPEC_divs-1, 1
  DL, (3*(DI_1-1) + 2), D, UY, 0
*ENDDO
DL, (3*(SPEC_divs-1) + 2), D, ALL, 0
SBCTRAN
*GET, NUM_NODES, NODE, 0, COUNT
*GET, NUM_ELEM, ELEM, 0, COUNT
NUM_CNT = 0
! ----------------------- DEAL WITH CRACK INFORMATION -----------------------
! Get the fixed nodes

*SET, NUM_FIXED, 1

*DIM, TEMPR, array, NUM_NODES

*DO, DI_1, 1, NUM_NODES, 1
    *GET, TEMP2, NODE, DI_1, D, UY
    *IF, TEMP2, LT, SPEC_height, THEN
        TEMPR(NUM_FIXED) = DI_1
        NUM_FIXED = NUM_FIXED + 1
    *ENDIF
*ENDDO

NUM_FIXED = NUM_FIXED - 1
*SET, PTR, 0

*DIM, FIXED, array, NUM_FIXED
*DIM, X_FIXED, array, NUM_FIXED

! Reorder the list to go from lowest to highest x position (left to right)

! **** Get the lowest x point

MIN_X = 2*SPEC_length

*DO, DI_2, 1, NUM_FIXED, 1
    *IF, NX(TEMPR(DI_2)), LT, MIN_X, THEN
        MIN_X = NX(TEMPR(DI_2))
    *ENDIF
*ENDDO

*DO, DI_1, 1, NUM_FIXED, 1
    FIXED(DI_1) = NODE(MIN_X, 0, 0)
    X_FIXED(DI_1) = MIN_X
    MIN_X = MIN_X + grid_x
*ENDDO

! Delete the lines and reinstate the loads on the nodes

*DO, DI_1, 1, SPEC_divs, 1
    DLDELE, (3*(DI_1-1) + 2), ALL
*ENDDO

! --------------------- DEFINE THE CNTs ---------------------
*IF, SPEC_wtp, GT, 0, THEN

  ! Define the number of materials
  TYPE, 5
  MAT, 5
  REAL, 5
  ESYS, 0

  ! Get the distance between CNTs
  CNT_dx = grid_x

  ! To be corrected

  ! Calculate the total number of CNTs needed (just the bonded length,
  ! excluding pre-crack)
  CNT_num = NINT((3 * SPEC_length / 5) / CNT_dx)

  ! To be corrected

  CNT_STARTNUM = (NUM_ELEM + 1)

ALLSEL, ALL

  *DO, DI_1, 1, CNT_num, 1
    NNODER = NODE(STARTD + (DI_1 - 2) * CNT_dx, 0, 0)
    N, (NUM_NODES + DI_1), NX(NNODER), NY(NNODER) - CNT_length, 0
    NNODER2 = NODE(NX(NNODER), NY(NNODER) - CNT_length, 0)
    D, (NNODER2), UX, 0
    D, (NNODER2), UY, 0
    EN, (CNT_STARTNUM + DI_1 - 1), (NNODER2), NNODER
  *ENDDO

  *GET, NUM_NODES, NODE, 0, COUNT
  *GET, NUM_ELEM, ELEM, 0, COUNT

  NUM_CNT = DI_1 - 2

*ENDIF

! Turn off all the CNTs

! ESEL, TYPE, 5 ! Select everything
! EKILL, ALL

! ---------------------- DEFINE THE RIGID BOUNDARIES -------------

FIX_N = NODE(SPEC_length, 0, 0)
D, FIX_N, UX, 0

ET, 3, COMBIN14
KEYOPT,3,1,0
KEYOPT,3,2,2
!KEYOPT,3,3,2

MPTEMP,,,,,,
MPTEMP,1,0
MPDATA,EX,3,,JOINT_moe
MPDATA,PRXY,3,,0.3
R,3,JOINT_moe/10,,,,

ESEL,ALL
*GET, NUM_ELEM2, ELEM, 0,COUNT
*GET, NUM_NODES2, NODE, 0,COUNT

TYPE,3
MAT,3
REAL,3
ESYS,0

*DIM,ELEM_FIXED,array,NUM_FIXED

*DO,DI_1,START,NUM_FIXED,1
  XPOP = NX(FIXED(DI_1))
  YPOP = NY(FIXED(DI_1))
  N,(NUM_NODES2 + DI_1-START+1),XPOP,YPOP,0,0,0,0
  EN,(NUM_ELEM2 + DI_1-START+1),FIXED(DI_1),(NUM_NODES2 + DI_1-START+1)
  ELEM_FIXED(DI_1) = (NUM_ELEM2 + DI_1-START+1)
*ENDDO

! Define the initial crack length (by deleting DOF on leftmost nodes.,

*DO,DI_1,1,(START-2),1
  FIXED(DI_1) = 0
*ENDDO

! -SOLVER-

! Set up solver parameters

*DIM,C3,array,2*MAX_COUNT
*DIM,P_LOAD,array,2*MAX_COUNT
*DIM,P_DISP,array,2*MAX_COUNT
*DIM,P_DEL,array,2*MAX_COUNT
*DIM,P_K1,array,2*MAX_COUNT
*DIM,P_TOUGH,array,2*MAX_COUNT
*DIM,KILLED_CNTS,array,2*MAX_COUNT
*SET,M_SLOPE,0
*SET, B_OFFSET, 0
*SET, TOT_SELECT, 0

/SOLU                    ! Enter SOLUTION

! solve for time 0 (no load)
*GET, APP_X, KP, 1000002, LOC, X
*GET, APP_Y, KP, 1000002, LOC, Y

APP_N = NODE(APP_X, APP_Y, 0)

D, APP_N, UY, 0
TIME, 0.00000000000001
T_DISP_Y = TEST_yinit

P_LOAD(1) = 0
P_DISP(1) = 0
P_DEL(1) = STARTD
P_K1(1) = 0
C3(1) = 0
P_TOUGH(1) = 0

ACEL, 0, 0, 0
NEQIT, ALLOW_ITER
CNVTOL, F, , FORCE_TOL, 2, 0.001
CNVTOL, U, , 0.01, Z, 0.001
NROPT, INIT

! You must explicitly set the Newton-Raphson option
RESCONTROL, DEFINE, NONE
! Use single-frame restart
TIMINT, ON
ANTYPE, TRANS
! SSTIF, ON
TRNOPT, FULL
! NLGEOM, ON
! Turns large-deflection effects on (disabled)

CUTCUTCONTROL, PLSLIMIT, 20

SAVE
SOLVE
SAVE
FINISH

! Solve for the initial extension (longer than increments to save time
before crack starts to propagate)
/SOLU
D, APP_N, UY, T_DISP

TIME, T_TIME
ANTYPE, REST
! nlgeo, on
PROPO = 0
! Start solving for crack
*DO,BIG_LOOP,2,300,1

! Check to see if the solution converged, and exit if not
*GET,DIDCON,ACTIVE,0,SOLU,CNVG
*STATUS,DIDCON
*IF,DIDCON,NE,0,THEN

! Find out if you need to cut down the step size based on
number of iterations (only works for the pre-crack)
*GET,NITERS,ACTIVE,0,SOLU,EQIT

/POST1 ! Enter POST1

! -------------- CALCULATE THE GLOBAL FRACTURE TOUGHNESS --------------

! Get the force acting on the application point
*GET,APP_F,NODE,APP_N,RF,FY
*STATUS,APP_F

! Get the C^1/3 value for this a
C3(BIG_LOOP) = EXP(log(abs(T_DISPY/APP_F))/3)

! Get the applied load
P_LOAD(BIG_LOOP) = APP_F

! Get the load point displacement
P_DISP(BIG_LOOP) = T_DISPY

! -------------- CHECK TO SEE IF CRACK SHOULD BE EXTENDED --------------
*SET,BREAK,0
*SET,BROKEN,0
! Find the left-most node that is still fixed

*DO, DI_1, 1, NUM_FIXED, 1
! *GET, TEMP2R, NODE, FIXED(DI_1), D, UY
*IF, FIXED(DI_1), NE, 0, EXIT
*ENDDO
DI_1 = DI_1 + 1

! Get the displacement and x-coordinates of the node and its left-adjacent

*GET, I_X, NODE, FIXED(DI_1), LOC, X
*GET, Z_X, NODE, APP_N, LOC, X
*GET, L_X, NODE, FIXED(DI_1-1), LOC, X

I_DX = UX(FIXED(DI_1))
Z_DX = UX(APP_N)
L_DX = UX(FIXED(DI_1-1))
P_DEL(BIG_LOOP) = (I_X + I_DX) - (Z_X + Z_DX)
DELTAX = (I_X + I_DX) - (L_X+L_DX)

! Get the y-displacement of the left-adjacent node and force on the constraint

L_Y = UY(FIXED(DI_1-1))
*GET, F_Y, ELEM, ELEM_FIXED(DI_1), SMISC, 1

! Calculate K1 at the fixed node
K1 = sqrt(-RVE_moe*(1/(DELTAX*SPEC_thick))*L_Y*F_Y)
P_K1(BIG_LOOP) = K1
K_TEMP = K1

*STATUS, K_TEMP

! Check to see how we should adjust the time step increments

*IF, (P_K1(BIG_LOOP-1)), GE, RVE_K1C, THEN
! Proportionally modify the load step increment (disp) to steady out the toughness
K_ERROR = 1 + 3*( (RVE_K1C*1.002)-K1)/(RVE_K1C*1.002)
TEST_yincs = TEST_yincs*(K_ERROR)
TEST_tincs = TEST_tincs*(K_ERROR)
! Limit the size (to prevent serious overshoot later)
*IF, TEST_yincs, GT, 5e-3, THEN
    TEST_yincs = 5e-3
    TEST_tincs = 5e-3
*ENDIF

*STATUS, TEST_yincs
*ENDIF

! See if crack should propagate
*IF, K1, GE, RVE_K1C, THEN
    TEST_yinc = TEST_yincs
    TEST_tinc = TEST_tincs

! Limit the size (to prevent serious overshoot later)
*IF, TEST_yinc, GT, 2e-3, THEN
    TEST_yinc = 2e-3
    TEST_tinc = 2e-3
*ENDIF

BREAK = 1
BROKEN = ELEM_FIXED(DI_1)

FIXED(DI_1-1) = 0
*SET, NEW_TEMP, FIXED(DI_1)
*STATUS, NEW_TEMP
*IF, PROPO, EQ, 0, THEN
    PROPO = BIG_LOOP
*ENDIF
*ENDIF

NUM_SELECT = 0

FINISH

! Calculate the global toughness
*IF, BIG LOOP, GE, 3, THEN
    *IF, P_DEL(BIG LOOP), NE, P_DEL(BIG LOOP-1), THEN
        M_SLOPE = (C3(BIG LOOP) - C3(BIG LOOP-1) ) / (P_DEL(BIG LOOP) - P_DEL(BIG LOOP-1))
    *ENDIF

    B_OFFSET = (((C3(BIG LOOP)) - M_SLOPE*(P_DEL(BIG LOOP))))
DELTA = 0

*IF, M_SLOPE, NE, 0, THEN
    DELTA = (B_OFFSET/M_SLOPE)
*ENDIF

*STATUS, DELTA

! IF, DELTA, LT, 0, THEN
DELTA = 0
!*ENDIF

P_TOUGH(BIG_LOOP) = 0

*IF,PROPO,NE,0,THEN

P_TOUGH(BIG_LOOP) = sqrt(abs((6*RVE_moe*P_LOAD(BIG_LOOP)*P_DISP(BIG_LOOP))/(2*SPEC_thick*(DELTA +P_DEL(BIG_LOOP)))))
*ENDIF

*ENDIF

! Start solving the next system

/SOLU                   ! Re-enter SOLUTION

! Increment all for the next load step
T_DISPY = T_DISPY + TEST_yinc
T_TIME = T_TIME + TEST_tinc

! Propagate the crack if specified beforehand
*IF,BREAK,EQ,1,THEN
    ESEL,ALL
    ESEL,S,,BROKEN
    EKILL,BROKEN
*ENDIF
*ELSEIF,DIDCON,EQ,0,EXIT
*ENDIF

ESEL,ALL

/SOLU                   ! Re-enter SOLUTION
D,APP_N,UY,T_DISPY
TIME,T_TIME
CNVTOL,F,,FORCE_TOL,2,0.001
CNVTOL,U,,0.01,2,0.001
NEQIT,ALLOW ITER
ANTYPE,,REST
!nlgeo,on
outres,all,none
outres,basic,all
CUTCONTROL,PLSLIMIT,20
SOLVE
SAVE
FINISH

BREAK = 0
BROKEN = 0

! Check EXIT condition

! Show the % completion for reference while running
PCTDONE = 100*(I_X-STARTD)/((3*SPEC_length/4)-STARTD)
*IF, I_X, GT, 3*SPEC_length/4, THEN
   PCTDONE = 100
*ENDIF
*STATUS, PCTDONE

*IF, I_X, GT, SPEC_length/2, EXIT
*ENDDO

! Post-processing output
!(save the load, displacement, crack opening, stress intensity factor, and
toughness in time history fields)

/POST26
FILE, 'file', 'rst', '.'
/UI,COLL,1
NUMVAR,200
SOLU,191,NCMIT
STORE, MERGE
FILLDATA,191,,,,1,1
REALVAR,191,191
FILLDATA,192,,,,0,0
FILLDATA,193,,,,1,0
FILLDATA,194,,,,-1,0
FILLDATA,195,,,,1,1
VARNAME,195,NSET

!
! Name: C3
! ID: 2
! Function: {C3}

FILLDATA,200,,,,2**(-100),0
VPUT,C3,200
REALVAR,2,200,,,,C3

FILLDATA,200,,,,2**(-100),0
VPUT,P_DISP,200
REALVAR,3,200,,,,P_DISP
FILLDATA,200,,,,2**(-100),0
VPUT,P_DEL,200
REALVAR,4,200,,,P_DEL
FILLDATA,200,,,2**(-100),0
VPUT,P_LOAD,200
REALVAR,5,200,,,P_LOAD
FILLDATA,200,,,2**(-100),0
VPUT,P_K1,200
REALVAR,6,200,,,P_K1
FILLDATA,200,,,2**(-100),0
VPUT,P_TOUGH,200
REALVAR,7,200,,,P_TOUGH
!
STORE,MERGE

/post1
! Animate (deflection)
PLDI,
!ANTIME,BIG_LOOP-1,0.1, ,1,2,TEST_tinit,T_TIME

!Save the data just in case
*CFOpen,data,csv
*VWRITE,P_DISP(1),P_DEL(1),P_LOAD(1),P_K1(1),P_TOUGH(1) ! Write array in given format to file "disp.dat" (f12.6,',f12.6,',f12.6,',f12.6,',f12.6)
*CFClose

! - END OF CODE -
APPENDIX B: RESULTS DATA TABLES

Neat epoxy data

<table>
<thead>
<tr>
<th>Displacement [mm]</th>
<th>Delamination [mm]</th>
<th>Load [N]</th>
<th>Crack Tip Gi [J/m²]</th>
<th>Toughness [MPa·m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>50.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
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<tr>
<td>0.675</td>
<td>49.961</td>
<td>78.368</td>
<td>20.268</td>
<td>0.655</td>
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<td>0.676</td>
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<td>78.403</td>
<td>20.287</td>
<td>0.655</td>
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<td>78.482</td>
<td>20.326</td>
<td>0.656</td>
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<tr>
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<td>49.961</td>
<td>78.584</td>
<td>20.362</td>
<td>0.657</td>
</tr>
<tr>
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<td>49.961</td>
<td>78.927</td>
<td>20.373</td>
<td>0.659</td>
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<tr>
<td>0.680</td>
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<td>79.069</td>
<td>20.411</td>
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<td>79.199</td>
<td>20.450</td>
<td>0.661</td>
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<tr>
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<td>49.961</td>
<td>79.005</td>
<td>20.462</td>
<td>0.661</td>
</tr>
<tr>
<td>0.683</td>
<td>49.961</td>
<td>79.147</td>
<td>20.496</td>
<td>0.662</td>
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<td>79.238</td>
<td>20.524</td>
<td>0.663</td>
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<td>79.551</td>
<td>20.548</td>
<td>0.664</td>
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<td>79.647</td>
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<td>0.665</td>
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<td>20.587</td>
<td>0.666</td>
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<td>79.325</td>
<td>20.599</td>
<td>0.665</td>
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| 0.933  | 49.958 | 94.418  | 7.496  | 0.844  |
| 0.948  | 49.957 | 96.044  | 7.775  | 0.858  |
| 0.963  | 49.956 | 97.668  | 8.053  | 0.873  |
| 0.978  | 49.956 | 99.293  | 8.328  | 0.887  |
| 0.993  | 49.955 | 100.641 | 8.537  | 0.899  |
| 1.008  | 49.954 | 102.270 | 8.810  | 0.913  |
| 1.023  | 49.954 | 103.898 | 9.081  | 0.928  |
| 1.038  | 49.953 | 105.527 | 9.351  | 0.942  |
| 1.053  | 49.952 | 106.598 | 9.553  | 0.953  |
| 1.068  | 49.952 | 108.223 | 9.822  | 0.967  |
| 1.083  | 49.951 | 109.847 | 10.090 | 0.982  |
| 1.098  | 49.950 | 111.223 | 10.290 | 0.993  |
| 1.113  | 49.950 | 112.850 | 10.556 | 1.008  |
| 1.128  | 49.949 | 114.475 | 10.821 | 1.022  |
| 1.143  | 49.948 | 116.100 | 11.086 | 1.037  |
| 1.158  | 49.948 | 117.168 | 11.286 | 1.047  |
| 1.173  | 49.947 | 118.796 | 11.549 | 1.062  |
| 1.188  | 49.946 | 120.425 | 11.812 | 1.076  |
| 1.203  | 49.946 | 122.055 | 12.184 | 1.091  |
| 1.218  | 49.945 | 123.402 | 12.563 | 1.102  |
| 1.233  | 49.944 | 125.024 | 13.068 | 1.117  |
| 1.248  | 49.944 | 126.645 | 13.568 | 1.131  |
| 1.263  | 49.943 | 128.266 | 14.065 | 1.146  |
| 1.278  | 49.942 | 129.389 | 14.435 | 1.156  |
| 1.293  | 49.942 | 131.019 | 14.925 | 1.171  |
| 1.308  | 49.941 | 132.648 | 15.412 | 1.185  |
| 1.323  | 49.940 | 134.277 | 15.896 | 1.200  |
| 1.338  | 49.940 | 135.565 | 16.258 | 1.211  |
| 1.353  | 49.939 | 137.188 | 16.739 | 1.226  |
| 1.368  | 49.938 | 138.811 | 17.217 | 1.240  |
| 1.383  | 49.937 | 140.435 | 17.693 | 1.255  |
| 1.398  | 49.937 | 141.602 | 18.048 | 1.265  |
| 1.413  | 49.936 | 143.228 | 18.521 | 1.280  |
| 1.428  | 49.935 | 144.855 | 18.992 | 1.294  |
| 1.443  | 49.935 | 146.480 | 19.462 | 1.309  |
| 1.458  | 49.934 | 147.748 | 19.814 | 1.320  |
| 1.473  | 49.933 | 149.373 | 20.282 | 1.334  |
| 1.488 | 49.933 | 150.544 | 20.632 | 1.345 |
| 1.503 | 49.941 | 151.890 | 10.546 | 1.357 |
| 1.518 | 49.941 | 153.149 | 10.770 | 1.368 |
| 1.533 | 49.940 | 154.503 | 10.993 | 1.380 |
| 1.548 | 49.939 | 157.116 | 11.436 | 1.404 |
| 1.563 | 49.938 | 158.378 | 11.656 | 1.415 |
| 1.578 | 49.938 | 159.730 | 11.876 | 1.427 |
| 1.593 | 49.937 | 160.992 | 12.095 | 1.439 |
| 1.608 | 49.937 | 162.343 | 12.313 | 1.450 |
| 1.623 | 49.936 | 163.607 | 12.531 | 1.462 |
| 1.638 | 49.935 | 166.221 | 12.965 | 1.485 |
| 1.653 | 49.934 | 167.569 | 13.373 | 1.497 |
| 1.668 | 49.934 | 168.835 | 13.802 | 1.509 |
| 1.683 | 49.933 | 170.142 | 14.020 | 1.520 |
| 1.698 | 49.933 | 171.449 | 14.239 | 1.532 |
| 1.713 | 49.932 | 172.756 | 14.457 | 1.544 |
| 1.728 | 49.931 | 175.370 | 14.893 | 1.567 |
| 1.743 | 49.930 | 176.678 | 15.111 | 1.579 |
| 1.758 | 49.930 | 177.985 | 15.329 | 1.590 |
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| 1.832 | 49.926 | 185.828 | 16.639 | 1.661 |
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| 1.892 | 49.924 | 191.056 | 17.511 | 1.707 |
| 1.907 | 49.923 | 193.671 | 17.948 | 1.731 |
| 1.922 | 49.922 | 194.978 | 18.166 | 1.742 |
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| 1.952 | 49.921 | 197.592 | 18.602 | 1.766 |
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| 1.982 | 49.920 | 200.206 | 19.039 | 1.789 |
| 1.997 | 49.919 | 202.821 | 19.475 | 1.813 |
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