To Mum and Dad,
for all your love and support
ABSTRACT

MICROMECHANICAL MODELLING OF DAMAGE AND FAILURE IN FIBRE REINFORCED COMPOSITES UNDER LOADING IN THE TRANSVERSE PLANE

TED J. VAUGHAN B. ENG

Fibre reinforced composites exhibit a gradual damage accumulation to failure, with a multitude of hierarchical dissipative mechanisms responsible for the deterioration of mechanical properties. In order to predict failure and gain a novel insight into the failure process, a micromechanics damage model was developed which predicts the onset and evolution of local microscopic damage mechanisms by representing the fibre and matrix phases discretely in the form of a Representative Volume Element (RVE). The micromechanical model was used to examine the influence of intra-ply properties on the mechanical behaviour of a high strength carbon fibre/epoxy composite under a range of loading scenarios in the transverse plane.

The Nearest Neighbour Algorithm (NNA) was initially developed in order to create statistically equivalent fibre distributions for high fibre volume fraction composites. This technique uses nearest neighbour distribution functions, measured from the microstructure of a high strength carbon fibre composite, to define inter-fibre distances in the RVE. The statistical distributions, characterising the resulting fibre arrangements, were found to be equivalent to those in the actual microstructure, allowing for an accurate representation of the microscopic stress state. Damage was implemented by using a Mohr-Coulomb material model to predict the onset and evolution of matrix plasticity, while a cohesive zone model was used to examine the effects of fibre-matrix debonding.

It was found that, under both transverse tensile and transverse shear loading, the fibre-matrix interface strength had a significant effect on the macroscopic strength, while the interface fracture energy had a marked effect on the strain to failure of the material. Interestingly, it was found that tailoring the properties of the fibre-matrix interface to a suitable level could promote the occurrence of certain sub-critical damage mechanisms, resulting in more favourable responses through a more effective dissipation of damage over the entire material microstructure. The presence of thermal residual stress had a significant influence on the interfacial stress state and, consequently, the onset of damage in the microstructure. However, its effect on the macroscopic strength was less pronounced. Under cyclic loading, the micromechanical model provided novel insight into the microscopic damage accumulation that forms prior to ultimate failure, and clearly highlighted the different roles that fibre-matrix debonding and matrix yielding play in forming the macroscopic response of the composite. Finally, the Composite Micromechanics (COMM) Toolbox was developed which provides efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. It is thought that the COMM Toolbox will advance multiscale/multilevel modelling strategies towards more practical industry based implementation, as it could prove useful in determining application specific properties for composite material systems by numerically carrying out various parameter studies on variables such as cure temperature and/or interface strength, for example.
Declaration

The substance of this thesis is the original work of the author and due reference and acknowledgement has been made, where necessary, to the work of others. No part of this thesis has already been submitted for any degree and is not being concurrently submitted in candidature for any degree.

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# Table of Contents

## Chapter 1

**Introduction and Objectives**  
1.1 Background .................................................. 1  
1.2 Motivation ................................................... 3  
1.3 Problem Description and Objectives .................. 5  
1.4 Overview of Thesis .......................................... 7

## Chapter 2

**Literature Review**  
2.1 Introduction .................................................. 9  
2.2 Damage and Failure in Composite Materials ........ 9  
   2.2.1 Damage Mechanisms in Fibre Reinforced Composites 10  
   2.2.2 Numerical Modelling of Damage and Failure in Composite Materials 13  
2.3 Micromechanics .............................................. 14  
   2.3.1 Periodic Homogenisation Approach .................. 15  
   2.3.2 Representative Volume Element ...................... 17  
2.4 Analysis of Fibre Distributions in Composite Microstructures 20  
   2.4.1 Spatial Point Patterns ................................ 21  
   2.4.2 Numerical Algorithms developed for Microstructure Generation 25  
   2.4.3 Experimental Microstructure Patterns .............. 27  
   2.4.4 Optimum size of the Representative Volume Element 29  
2.5 Effect of the Constituent Materials on Mechanical Behaviour 30  
   2.5.1 Epoxy Matrix Behaviour .............................. 31  
   2.5.2 Fibre-Matrix Interface ................................ 35  
   2.5.3 Thermal Residual Stress .............................. 39  
2.6 Micromechanics Damage Models ......................... 41  
2.7 Discussion of Literature Review ......................... 47  
   2.7.1 Introduction ............................................ 47  
   2.7.2 Damage and Failure in Composite Materials .... 47  
   2.7.3 Micromechanical Modelling of Composites ......... 48  
   2.7.4 Analysis of Fibre Distribution in Composite Microstructures 49  
   2.7.5 Effect of Constituent Materials on Mechanical Behaviour 50  
   2.7.6 Micromechanics Damage Models ...................... 52
Chapter 3
Generating Statistically Equivalent Fibre Distributions for High Strength Composites

3.1 Introduction 55
3.2 Experimental Characterisation of Fibre Arrangement 56
  3.2.1 Sample Preparation 57
  3.2.2 Digital Image Analysis 57
3.3 Statistical Characterisation of CFRP Microstructure 58
  3.3.1 Nearest Neighbour Distributions 59
  3.3.2 Radial Distribution Function 60
  3.3.3 Second-Order Intensity Function 61
3.4 Nearest Neighbour Algorithm (NNA) 62
  3.4.1 Algorithm Description 62
3.5 Statistical Characterisation of Nearest Neighbour Algorithm 66
  3.5.1 Nearest Neighbour Distributions 68
  3.5.2 Radial Distribution Function 69
  3.5.3 Second-Order Intensity Function 70
  3.5.4 Fibre Volume Fraction 71
  3.5.5 Model Generation Time 72
3.6 Prediction of Effective Properties 72
  3.6.1 Periodic Boundary Conditions 73
  3.6.2 Homogenisation Procedure 77
  3.6.3 Resulting Effective Properties 80
3.7 Concluding Remarks 82

Chapter 4
Micromechanical Modelling of the Transverse Damage Behaviour in Fibre Reinforced Composites

4.1 Introduction 85
4.2 Finite element modelling 87
  4.2.1 Generation of micromechanical models 88
  4.2.2 Material Behaviour 90
4.3 Results 96
  4.3.1 Microscopic stress state after thermal cool-down 96
  4.3.2 Fibre-Matrix Debonding 98
  4.3.3 Damage Accumulation under Cyclic Loading 107
4.4 Concluding Remarks 111
### Chapter 5

**Micromechanical Modelling of Transverse Shear Deformation in Fibre Reinforced Composites**

- 5.1 Introduction 113
- 5.2 Finite element modelling 115
  - 5.2.1 Generation of micromechanical models 115
  - 5.2.2 Material Behaviour 117
- 5.3 Results 117
  - 5.3.1 Interfacial stress state under transverse shear loading 117
  - 5.3.2 Fibre-Matrix Debonding 121
  - 5.3.3 Effect of Thermal Residual Stress on Failure Surface 135
- 5.4 Concluding Remarks 139

### Chapter 6

**A MATLAB Micromechanics Toolbox for Composite Materials**

- 6.1 Introduction 141
- 6.2 Development of the COMM Toolbox 142
  - 6.2.1 Main COMM Toolbox GUI 143
  - 6.2.2 Pre-processing Abaqus Input Files for Non-Linear Analysis 150
  - 6.2.3 Post-Processing Abaqus Results 155
- 6.3 Case Studies using COMM Toolbox 156
  - 6.3.1 Case Study A: Effect of fibre volume fraction on transverse behaviour 157
  - 6.3.2 Case Study B: Effect of fibre distribution on transverse behaviour 164
- 6.4 Concluding Remarks 170

### Chapter 7

**Conclusions and Recommendations for Future Work**

- 7.1 Introduction 173
- 7.2 Concluding Remarks 173
  - 7.2.1 Nearest Neighbour Algorithm 173
  - 7.2.2 Micromechanical Behaviour under Loading in the Transverse Plane 174
  - 7.2.3 Composite Micromechanics Toolbox 178
- 7.3 Recommendations for Future Work 179
  - 7.3.1 Micromechanical Modelling 179
  - 7.3.2 Microscale Experimental Characterisation 182

References 185
### Appendix A

**Model Parameter Analysis**

- A.1 Introduction
- A.2 Mesh Sensitivity Analysis
- A.3 Viscosity Co-efficient

### Appendix B

**MATLAB and Python Codes**

- B.1 Introduction
- B.2 Nearest Neighbour Algorithm
- B.3 Hard-Core Model
- B.4 Python Script to interface between MATLAB and ABAQUS
List of Figures

Chapter 1

Figure 1.1: Manufacturing process involved in high strength composite materials......................................................................................................................... 3

Figure 1.2: Hierarchical nature of damage in a composite from intra-ply level damage (from Hobbiebrunken et al. (2006)), ply level damage in 90° and 45° off-axis plies (from Lafarie-Frenot et al. (2001)) and laminate level. ...................................................................... 4

Figure 1.3: Idealised square Representative Volume Element................................................. 6

Chapter 2

Figure 2.1: Damage mechanisms due to loading in the transverse plane (a) transverse tensile loading (b) transverse compressive loading and (c) transverse shear loading................................................................. 11

Figure 2.2: Damage mechanisms due to loading in the fibre direction (a) fibre fracture due to tensile loading and (b) fibre buckling due to compressive loading and (c) failure due to longitudinal shear loading. .................................................................................................................. 12

Figure 2.3: Delamination in a laminate configuration under (a) tensile loading as a result of transverse ply cracking and (b) subsequent buckling under compressive loading.................................................. 13

Figure 2.4: Concept of replacing discrete cracking process with an effective continuum. ................................................................. 14

Figure 2.5: Macroscopically homogenous material characterised by a heterogeneous microstructure associated with the point P. ...................... 15

Figure 2.6: Periodic boundary conditions applied to a microscopically heterogeneous material. .............................................................................................. 16

Figure 2.7: Regular fibre arrays and their associated periodic fibre unit cells: (a) square and (b) hexagonal periodic fibre arrays......................... 18

Figure 2.8: Micrograph of a carbon fibre composite showing spatial arrangement of fibres................................................................. 19
Figure 2.9: Spatial point patterns exhibiting a (a) random distribution (Poisson point field) (b) regular distribution (c) dispersed distribution (hard-core point field) and (d) a clustered distribution ................................................. 22

Figure 2.10: Radial area of influence for calculating the second-order intensity function and radial distribution function ............................................................. 23

Figure 2.11: Fibre stirring procedure (from Melro et al. (2008)) ................................................ 26

Figure 2.12: Second order intensity function showing varying fibre patterns (reproduced from Pyrz (1994b)) ......................................................................................... 27

Figure 2.13: Direct microstructure approach (from Trias (2005)) ........................................ 28

Figure 2.14: (a) Variation of local fibre volume fraction (from Silberschmidt (2008)) and (b) Convergence of local fibre volume fraction with window size (reproduced from Silberschmidt (2008)) ........................................ 29

Figure 2.15: Transverse tensile response of carbon fibre/epoxy and glass fibre/epoxy composites (from O’Higgins et al. (2009)) ........................................ 31

Figure 2.16: Mohr-Coulomb yield locus in the Mohr stress space ................................................. 33

Figure 2.17: Yield surfaces in the principal stress space: (a) Mohr-Coulomb (b) Von-Mises and (c) Drucker-Prager ......................................................................................... 34

Figure 2.18: In-situ experimental failure observation of carbon fibre/epoxy composites by Hobbiebrunken et al. (2006) having a (a) strong fibre-matrix interface and (b) weak fibre-matrix interface ........................................ 37

Figure 2.19: (a) Initiation of debond in a cross-ply laminate subject to transverse loading (b) Coalescence of interface cracks to form transverse crack ........................................ 38

Figure 2.20: In-Situ SEM observation of fibre-matrix debonding due a transverse shear load applied during a double notch shear test ................................. 38

Figure 2.21: Interfacial damage caused by thermal residual stress (from Gentz et al. (2004)) .................................................................................................................. 40

Figure 2.22: Effect of thermal residual stress on fracture surface (a) biaxial transverse normal loading and (b) transverse normal/shear loading ............................................. 41

Figure 2.23: Bi-linear traction separation law governing behaviour of a CZM ................................................................................................................................. 43

Figure 2.24: Finite element discretisation where interface elements are located at the fibre-epoxy interface and between continuum elements in the epoxy (from Cid Alfaro et al. (2010)) ............................................. 44

Figure 2.25: (a) Transverse tensile deformation in a fibre reinforced rubber modified epoxy composite (load applied in the vertical direction) (from Canal et al. (2009)) and (b) transverse compressive deformation of a fibre reinforced epoxy composite with a strong fibre matrix interface (from González & Llorca (2007a)) ........................................ 46
Figure 2.26: Transverse shear deformation of a carbon fibre/epoxy composite for (a) a strong fibre-matrix interface and (b) a weak fibre matrix interface (legend indicates plastic strain), (from Totry et al. (2008a)) ................................................................. 46

Chapter 3

Figure 3.1: Sample image chosen for analysis (320µm × 240µm), (a) actual micrograph, (b) computed microstructure based on a colour threshold algorithm ........................................................................ 58

Figure 3.2: Fibre diameter distribution fit to a lognormal distribution curve ................................................................. 59

Figure 3.3: Experimentally measured nearest neighbour distances (a) 1st nearest neighbour distribution function (b) 2nd nearest neighbour distribution function ........................................................................ 60

Figure 3.4: Radial distribution function for the composite ................................................................. 61

Figure 3.5: Second-order intensity function ............................................................................................... 62

Figure 3.6: 'Adjusted' measure of the nearest neighbour distribution function ........................................................................ 63

Figure 3.7: Logistic distributions fit to the 'adjusted' measures of the (a) 1st nearest neighbour distribution and (b) 2nd nearest neighbour distribution ........................................................................ 63

Figure 3.8: Assigning a fibre’s nearest neighbour ............................................................................................... 64

Figure 3.9: Assigning a fibre's second nearest neighbour ............................................................................................... 65

Figure 3.10: Nearest neighbour being assigned for a subsequent fibre ............................................................................................... 65

Figure 3.11: NNA in the process of generating a sample microstructure measuring 165µm ×165µm with snapshots taken at (a) 10% Vf (b) 20% Vf (c) 30% Vf (d) 40% Vf (e) 50% Vf and (f) 60% Vf ........................................................................ 66

Figure 3.12: (a) Generated distribution using Nearest Neighbour Algorithm (b) Periodic hexagonal fibre array ............................................................................................... 68

Figure 3.13: Micrograph from experimental CFRP sample ............................................................................................... 68

Figure 3.14: (a) 1st Nearest neighbour distances (b) 2nd Nearest neighbour distances ............................................................................................... 69

Figure 3.15: Radial distribution function ............................................................................................... 70

Figure 3.16: Second-order intensity function ............................................................................................... 71

Figure 3.17: Fibre volume fraction size study ............................................................................................... 72

Figure 3.18: Periodic boundary conditions applied to an RVE ............................................................................................... 74

Figure 3.19: Periodic boundary conditions for the transverse tensile loading case as applied (a) in the 2-direction and (b) in the 3-direction ............................................................................................... 75
List of Figures

Figure 3.20: Periodic boundary conditions and resulting deformation for transverse shear................................................................. 75
Figure 3.21: Periodic boundary conditions for longitudinal tension............ 76
Figure 3.22: Periodic boundary conditions applied to an RVE to determine the in-plane shear modulus ................................................. 77
Figure 3.23: Deformation of an RVE under in-plane shear loading ............. 77
Figure 3.24: Surface based homogenisation for an applied (a) normal displacement and (b) shear displacement .................................. 79
Figure 3.25: Effective properties of the numerically generated microstructures in (a) the longitudinal direction and (b) the transverse and in-plane directions (Experimental values (denoted by ‘Exp’) are taken from O’Higgins et al. (2008)) ...................... 81

Chapter 4

Figure 4.1: In-situ experimental failure observation of carbon fibre/epoxy composites (from Hobbiebrunken et al. (2006)). ................................. 86
Figure 4.2: Periodic boundary conditions applied to an RVE simulating the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case. ........................................................................ 89
Figure 4.3: Traction-separation law governing behaviour of cohesive elements ......................................................................................... 94
Figure 4.4: Interfacial Normal Stress (INS) following the thermal cool-down from cure temperature................................................................. 97
Figure 4.5: Interfacial Shear Stress (ISS) following the thermal cool-down from cure temperature ................................................................. 98
Figure 4.6: Transverse fracture behaviour of an RVE generated by the NNA for various interfacial strengths (Experimental results from O’Higgins et al. (2009)) .................................................................................. 99
Figure 4.7: (a) Damaged cohesive elements following the thermal cool-down in an RVE with a weak fibre-matrix interface (b) Initiation and propagation of interface cracks due to thermal residual stress (Note: a deformation scale factor of 20 has been used in the above images). ................................................................................ 100
Figure 4.8: Interfacial damage due to thermal residual stress (from Gentz et al. (2004)). .................................................................................. 100
Figure 4.9: Progression of damage through an RVE with an interfacial strength of 15 MPa for the (a) Mechanical Loading case (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 15 MPa (Note: a deformation scale factor of 5 has been used in the above images) .................................................................................. 102
Figure 4.10: Progression of damage through an RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 60MPa (Note: a deformation scale factor of 5 has been used in the above images). .......................................................... 104

Figure 4.11: Progression of damage through another RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case (Note: a deformation scale factor of 5 has been used in the above images). .......................................................... 105

Figure 4.12: Effect of interfacial fracture energy on transverse response (Experimental results from O’Higgins et al. (2009)). ............................. 107

Figure 4.13: (a) Experimental transverse tensile cyclic loading of HTA/6376 (from O’Higgins 2007). (b) Transverse tensile cyclic loading predicted using micromechanical modelling. ................... 109

Figure 4.14: The response of an RVE subject to successive tensile and compressive loading and microscopic damage accumulation observed (a) following initial tensile loading (Load Point A) (b) following unloading from tensile stress state (Load Point B) and (c) following subsequent compressive loading (Load Point C) (Note: a deformation scale factor of 5 has been used in the above images). .......................................................... 111

Chapter 5

Figure 5.1: In-Situ SEM observation of fibre-matrix debonding due a transverse shear load applied during a double notch shear test (from Hinz et al. (2009)) ................................................................................. 114

Figure 5.2: Periodic boundary conditions applied to RVE to simulate transverse shear loading for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case. .................................................. 116

Figure 5.3: Transverse shear deformation of an RVE showing directions of the maximum (σ₁) and minimum (σ₃) principal stresses. .................. 118

Figure 5.4: Distribution of Interfacial Normal Stress around (a) Fibre A₀ and (b) Fibre B₀. .............................................................................. 119

Figure 5.5: Distribution of Interfacial Shear Stress around (a) Fibre A₀ and (b) Fibre B₀. ............................................................................... 121

Figure 5.6: Transverse shear behaviour of an RVE generated by the NNA for both the ML and TML cases for different interface strengths. .................. 122
Figure 5.7: Progression of damage through an RVE with an interfacial strength of 15MPa for the (a) Mechanical Loading case (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 15MPa (Note: a deformation scale factor of 2 has been used in the above images). ................................................................. 124

Figure 5.8: Progression of damage through an RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 60MPa (Note: a deformation scale factor of 2 has been used in the above images). .................................................................................................... 126

Figure 5.9: (a) Progression of damage through an RVE with an interfacial strength of 120 MPa for the Mechanical Loading case and (b) stress-strain response for an interfacial strength of 120 MPa (Note: a deformation scale factor of 2 has been used in the above images). ......................................................................................... 128

Figure 5.10: Effect of interface strength on transverse shear behaviour of a ‘matrix rich’ RVE. ................................................................................................................................. 130

Figure 5.11: Progression of damage for the Mechanical Loading case for an interfacial strength of 120 MPa through a modified ‘matrix rich’ RVE and (b) stress-strain response for an interfacial strength of 120MPa (Note: a deformation scale factor of 2 has been used in the above images). ....................................................................................... 131

Figure 5.12: Final fracture path of the modified ‘matrix rich’ RVE for an interfacial strength of 60 MPa for the (a) ML case and (b) TML case (Note: a deformation scale factor of 2 has been used in the above images). ..................................................................................... 132

Figure 5.13: Effect of interface fracture energy on the transverse shear response. ................................................................................................................................. 133

Figure 5.14: Progression of damage through an RVE with different fracture energies: (a) $\Gamma=2.5$ J/m$^2$ (b) $\Gamma=100$ J/m$^2$ and (c) stress-strain response for different fracture energies (Note: a deformation scale factor of 2 has been used in the above images). ..................................................................................... 134

Figure 5.15: Combined transverse normal and shear displacements applied to an RVE. ................................................................. 135

Figure 5.16: Failure surface generated by micromechanical models using combined transverse normal and shear loading regime. .................... 137

Chapter 6

Figure 6.1: Initialising the COMM Toolbox through the main MATLAB window. .................................................................................................. 143
List of Figures

Figure 6.2: Main GUI of the COMM Toolbox. ......................................................... 144
Figure 6.3: Fibre distributions available in the COMM Toolbox: (a) Nearest Neighbour Algorithm (b) Hard-Core Model (c) Hexagonal Periodic Array and (d) Square Periodic Array. .................... 145
Figure 6.4: NNA Properties GUI. ................................................................. 146
Figure 6.5: GUI for statistical analysis of fibre distribution. ................................. 147
Figure 6.6: (a) Laminate Properties GUI and (b) Material Properties GUI ............ 148
Figure 6.7: Tasks carried out by the COMM Toolbox to determine effective properties for an RVE. ............................................................................ 149
Figure 6.8: ABAQUS Analysis GUI for pre-processing files for non-linear analysis.......................................................... 150
Figure 6.9: Material Properties GUI................................................................ 151
Figure 6.10: Mesh Properties GUI. ............................................................... 152
Figure 6.11: (a) Loads/Boundary Conditions GUI (b) Boundary conditions applied to an RVE ................................................................................... 152
Figure 6.12: Analysis Outputs GUI. ............................................................. 153
Figure 6.13: Submitting jobs to parallel computing resources using the COMM Toolbox.................................................................................. 155
Figure 6.14: GUI for post-processing Abaqus output database files. .................... 155
Figure 6.15: Fibre distributions generated by the COMM Toolbox for (a) $V_f = 20\%$ (b) $V_f = 40\%$ and (c) $V_f = 59\%$. ......................................................... 158
Figure 6.16: (a) 1st Nearest Neighbour Distribution function and (b) 2nd Nearest Neighbour Distribution function for distributions generated. ................................................................................. 159
Figure 6.17: Boundary conditions applied to an RVE ($V_f = 20\%$) for the combined transverse compressive and shear loading case. ..................... 160
Figure 6.18: Effect of fibre volume fraction on transverse failure surface for interface dominated failure. ............................................................................. 162
Figure 6.19: Final deformation for a loading ratio of $\delta_n/\delta_t = -2$ in RVEs where (a) $V_f = 20\%$ and (b) $V_f = 59\%$. ................................................................................. 162
Figure 6.20: Effect of fibre volume fraction on transverse failure surface for matrix dominated failure.................................................................................... 163
Figure 6.21: Final deformation for a loading ratio of $\delta_n/\delta_t = -1$ in RVEs where (a) $V_f = 20\%$ and (b) $V_f = 59\%$. ................................................................................. 163
Figure 6.22: 1st and 2nd Nearest Neighbour Distribution (NND) Parameters governing inter-fibre distances for fibre volume fractions of 59% and 52% generated by the NNA. ................................................................. 164
Figure 6.23: Fibre distributions with a 52% fibre volume fraction generated by the COMM Toolbox using the (a) Nearest Neighbour Algorithm (b) Hard-Core Model (c) Hexagonal Periodic Array and (d) Square Periodic Array. ......................................................... 165
List of Figures

Figure 6.24: Lognormal distributions governing fibre diameter distributions in the NNA................................................................. 166

Figure 6.25: RVE generated by the COMM Toolbox assuming the fibre diameter distribution NNA-VD. .............................................. 166

Figure 6.26: Transverse failure surface for each of the fibre distributions under consideration...................................................... 167

Figure 6.27: Effect of fibre distribution on the transverse tensile response of the material............................................................. 169

Figure 6.28: Progression of fibre-matrix debonding and matrix yielding due to transverse tensile loading the (a) Hexagonal Periodic array and (b) Square Periodic array. ...................................................... 169

Figure 6.29: Progression of damage in an RVE with a variable fibre diameter. ........................................................................ 170

Chapter 7

Figure 7.1: Multi-Ply RVE to analyse progression of intra-ply damage to the inter-ply region........................................................... 180
List of Tables

Chapter 3

Table 3.1: Constituent Material Properties ................................................................. 80

Chapter 4

Table 4.1: Constituent Thermo-Mechanical Properties ............................................... 91

Chapter 5

Table 5.1: Mohr-Coulomb Parameters....................................................................... 117
Table 5.2: Strength values predicted by micromechanical models............................ 138
Nomenclature

The nomenclature defined below relates to Chapters 3 to 7. The symbols used in Chapter 2 depend on their original use in the literature and are clearly defined.

Upper Case

A  Area of Representative Volume Element
C_{ijkl}  Stiffness tensor
D  Cohesive damage variable
D_i  Regularised cohesive damage variable
E_{ij}  Elastic modulus
E_{22}^0  Initial transverse modulus
E_{22}^i  Transverse modulus upon i^{th} loading cycle
G_{ij}  Shear modulus
G(r)  Radial distribution function
I_k(r)  Indicator function
J_i  Deviatoric stress invariants
K(r)  Second-order intensity function
K^0  Initial elastic stiffness
L  Side length of Representative Volume Element
N  Number of fibres
N_a  Number of fibres per unit area
S_{ijkl}  Compliance tensor
S_{23}  Transverse shear strength
S_{22}^T  Transverse tensile strength
Nomenclature

$S_{22}^C$  Transverse compressive strength

T  Temperature

$T_G$  Glass transition temperature

$U_v$  Dilatational energy density

V  Volume of Representative Volume Element

$V_f$  Fibre volume fraction

$V_k$  Element volume

Lower Case

c  Cohesion stress

d_f  Fibre diameter

d_{ij}  Damage tensor

$f_n$  Normal force

$f_t$  Tangential force

k  Element number

n  Number of elements around fibre circumference

$n_i$  Active control node

r  Radial distance

$r_f$  Fibre radius

$t^o$  Cohesive interface strength

$t_n$  Interfacial normal stress

$t_n^e$  Elastic prediction of interfacial normal stress

$t_n^o$  Interfacial normal strength

$t_s$  Interfacial shear stress

$t_s^e$  Elastic prediction of interfacial shear stress
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau$</td>
<td>Interfacial shear strength</td>
</tr>
<tr>
<td>$\mathbf{u}$</td>
<td>Nodal displacement vector</td>
</tr>
<tr>
<td>$w_k$</td>
<td>Edge-correction function</td>
</tr>
</tbody>
</table>

### Greek Letters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_n$</td>
<td>Coefficient of thermal expansion</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Fracture energy</td>
</tr>
<tr>
<td>$\gamma_{ij}$</td>
<td>Shear strain</td>
</tr>
<tr>
<td>$\bar{\gamma}_{ij}$</td>
<td>Average shear strain</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Size of Representative Volume Element</td>
</tr>
<tr>
<td>$\delta_{m}$</td>
<td>Effective mixed-mode cohesive displacement</td>
</tr>
<tr>
<td>$\delta_{m}^{\text{max}}$</td>
<td>Maximum effective mixed-mode cohesive displacement</td>
</tr>
<tr>
<td>$\delta_{m}^{\prime}$</td>
<td>Effective mixed-mode cohesive displacement at failure</td>
</tr>
<tr>
<td>$\delta_{m}^{\ast}$</td>
<td>Effective mixed-mode cohesive displacement at the onset of damage</td>
</tr>
<tr>
<td>$\delta_n$</td>
<td>Normal displacement</td>
</tr>
<tr>
<td>$\delta_n^{\prime}$</td>
<td>Normal cohesive displacement at failure</td>
</tr>
<tr>
<td>$\delta_s$</td>
<td>Shear displacement</td>
</tr>
<tr>
<td>$\delta_s^{\prime}$</td>
<td>Shear cohesive displacement at failure</td>
</tr>
<tr>
<td>$\varepsilon_{ij}$</td>
<td>Strain</td>
</tr>
<tr>
<td>$\bar{\varepsilon}_{ij}$</td>
<td>Average strain</td>
</tr>
<tr>
<td>$\varepsilon_{22}^{\prime}$</td>
<td>Transverse plastic strain</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Viscosity coefficient</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>$\sigma_{ij}$</td>
<td>Stress</td>
</tr>
</tbody>
</table>
Nomenclature

\( \sigma_n \)  Normal stress
\( \sigma_1 \)  Maximum principal stress
\( \sigma_2 \)  Intermediate principal stress
\( \sigma_3 \)  Minimum principal stress
\( \sigma_C \)  Compressive strength
\( \sigma_T \)  Tensile strength
\( \sigma_{ij} \)  Average stress
\( \tau_{ij} \)  Shear stress
\( \overline{\tau}_{ij} \)  Average shear Stress
\( \phi \)  Internal friction angle
Chapter 1

Introduction and Objectives

1.1 Background

Polymer matrix composites are strong, lightweight, engineered materials consisting of high performance reinforcing fibres embedded in a polymeric matrix. The fibres, which exhibit high strength and stiffness, are the load bearing phase of the material and are commonly made from carbon or glass. In contrast, the polymeric matrix phase is more compliant and its function is to adhere the fibres together, giving the material its shape, while also allowing stress transfer between individual reinforcements. Fibre reinforced composite materials are used extensively in the aerospace industry and are finding increasing applications in other industries such as automotive, civil and energy. Their high strength and stiffness coupled with their low weight make them attractive materials, especially in transport applications where fuel savings can be realised.

Much of the development in the field of composite materials has been driven by the rapid expansion of the commercial aviation sector. Since the mid-eighties, their application towards commercial aviation has seen an increasing number of secondary structures, such as engine cowlings, leading/trailing edge panels and vertical tail fins, being manufactured with both carbon and glass fibre/epoxy composites. Towards the end of the last century, composite materials accounted for almost 20% of both the Boeing 777 and Airbus A330 airframe structures (by weight). Recently, increasing uncertainty of fuel prices coupled with pressure on airlines to reduce CO$_2$ emissions has
seen a transition in the use of composite materials from secondary to primary load-bearing structures. The new Boeing 787 represents a breakthrough in commercial aircraft design as it adopts an innovative all composite fuselage, which promises lower running costs. Similarly, the upcoming Airbus A350 also plans a predominantly composite fuselage as well as composite wing and empennage sections. Meanwhile, Bombardier’s CSeries aircraft, although not incorporating a composite fuselage, utilizes fully composite wing sections which have been developed at their Belfast facility. This new generation of efficient aircraft sees composite materials accounting for upwards of 50% of the airframe structure (by weight). Realising such large composite structures presents a number of challenges, as accurate predictive tools and extensive physical testing are needed in both the design and certification phases of production. Also, the fabrication of such large composite assemblies requires advanced large scale manufacturing and processing techniques.

For high strength applications, the manufacturing process of a fibre reinforced composites involves assembling structures using thin plies of unidirectional fibres which have been pre-impregnated with the uncured epoxy. Depending on the manufacturing process, the individual plies are successively laid down, either by hand or using automated tape laying machines, to form a laminated or layered structure. Importantly, the successive nature of the individual plies in composite structures means that, unlike other monolithic materials, the strength and stiffness of the component can be tailored to match the anticipated structural demands. The final stage of the manufacturing process requires the curing of the epoxy which is carried out in an autoclave under elevated temperature and pressure. This consolidates the individual plies into a single laminate configuration, as shown in Fig. 1.1.
1.2 Motivation

Despite the fact that composite materials are being used in primary load-bearing aircraft structures, current design practices and strength predictions are not fully mature and, surprisingly, there is a lack of supporting evidence that many of the ply level failure criteria developed thus far could provide meaningful and accurate predictions for composite materials beyond a limited range of circumstances (Hinton & Soden 1998). Failure in composite materials is a consequence of phenomena taking place at (or below) the microscopic scale and the difficulties associated with accurately predicting material failure is due to the inherent heterogeneity at this scale, i.e. the existence of two phases in the material microstructure with vastly different constitutive behaviour. Local microscopic damage mechanisms, including fibre fracture, fibre-matrix debonding and matrix micro-cracking, contribute to gradual ply degradation. These local phenomena are rarely independent events as, through the process of damage accumulation, these local failures coalesce and traverse higher length scales until ultimately leading to macroscopic failure.

Thus, fracture is a multiscale process involving the interaction of a multitude of simultaneously occurring local damage mechanisms. This multiscale nature of damage is shown schematically in Fig. 1.2, where damage initiates at the ‘intra-ply level’ through a number of local intra-ply failure mechanisms. At this level, fibre-matrix debonding occurs at the interface and, due to stress redistribution, matrix
Introduction and Objectives

yielding/cracking occurs in adjoining matrix regions which in turn forms a transverse crack at the ‘ply level’. From the ‘ply level’ the stress concentration at the tip of the transverse crack causes delamination at the ply boundary, as shown, and also results in stress redistribution to neighbouring plies which can bring about earlier failure through fibre fracture, thus affecting the composite on the ‘laminate level’.

![Hierarchical nature of damage in a composite](image)

Figure 1.2: Hierarchical nature of damage in a composite from intra-ply level damage (from Hobbiebrunken et al. (2006)), ply level damage in 90° and 45° off-axis plies (from Lafarie-Frenot et al. (2001)) and laminate level.

Previously, commercial design practices relied heavily on costly experimental tests on coupons and structural elements, as well as generous safety margins to accommodate material uncertainty. To advance the use of composite materials and maximise their application, predictive capabilities are advancing as an effective means to reduce certification costs as the industry moves towards certification by analysis supported by test and demonstration. The current state-of-the-art in finite element modelling of damage and failure in composite structures uses continuum damage mechanics to predict ply degradation, where various internal damage mechanisms are generalised to create a damage tensor, upon which the mechanical properties depend. While these models allow for an adequate prediction of experimental non-linear behaviour, they still rely on non-physical material parameters, such as plasticity/damage coupling factors, to account for non-linear behaviour (O'Higgins et al. 2009). Moreover, these models do not consider the microscopic development of failure and, consequently, offer little insight into why composites fail.
In order to predict microscopic damage accumulation and its effect on the macroscopic structure, multiscale modelling approaches have begun to appear in the literature. In particular, computational micromechanics has been shown to provide a suitable framework to present detailed predictions of local deformation mechanisms in heterogeneous materials (González & Llorca 2007b). At a fundamental level, any loading situation on a composite material results in an interaction between the constituents and so, representing the fibre and matrix phases discretely in micromechanical simulations facilitates a better understanding of their influence on macroscopic and structural behaviour for both material scientists and engineers. Early computational micromechanics models resolved local stress and strain fields to analyse the effect of particle size, shape and distribution (Brockenbrough et al. 1991), thus establishing quantitative relations between the microstructure morphology and physical properties at higher length scales. Recent advances in fracture modelling means discrete microscale damage processes can be simulated through, for example, the use of cohesive zone models at particle interfaces. These, coupled with non-linear constitutive models to describe behaviour of individual phases, enable the prediction of diffuse and complex fracture patterns.

1.3 Problem Description and Objectives

This thesis outlines the development of a micromechanics damage model which examines the failure behaviour of a carbon fibre/epoxy composite under a range of loading scenarios in the transverse plane. The accuracy of micromechanics based failure predictions relies heavily upon the definition of a suitable Representative Volume Element (RVE). The RVE should take a form similar to that shown in Fig. 1.3, where the fibres of diameter, \( d_f \), are distributed within a square domain, \( A \), having a side of length, \( L \). The distribution of fibres within the RVE should be statistically equivalent to the actual experimental microstructure (Grufman & Ellyin 2008). A number of numerical and experimental strategies have been proposed to define suitable fibre arrangements in the RVE, however, these strategies have a number of shortcomings. Many numerical approaches have not been statistically verified against actual microstructures, while experimental approaches present a number of difficulties when it comes to applying suitable periodic boundary conditions. Thus, the first objective of this thesis can be identified as follows,
1) To develop a combined experimental-numerical approach to generate statistically equivalent fibre distributions. The method should be verified against a number of mechanical and statistical criteria to ensure it is robust and accurate, so it can be used in subsequent micromechanics damage simulations.

As was shown in Fig. 1.2, the failure behaviour of transverse plies has a significant influence on the overall failure of composite laminates. Transverse failure often occurs early in the loading history and as a result is one of the limiting design criteria in composite structures. Consequently, much of the work presented in this thesis will focus upon the damage behaviour under transverse tensile or transverse shear loading. The damage and fracture behaviour of composite materials under loading in the transverse plane has been shown to depend upon numerous contributing factors, such as constituent properties, interfacial properties, local fibre distribution and the presence of thermal residual stresses. While a number of micromechanical studies have examined failure under transverse tensile loading, this thesis will further investigate the transverse damage behaviour, with a particular focus on the effects of thermal residual stress and fibre-matrix debonding. Meanwhile, very few studies exist which examine the micromechanical behaviour of composites under transverse shear loading and so, two further objectives of this work may be identified as follows,

2) To examine the damage behaviour of the carbon fibre/epoxy composite under transverse tensile loading and determine the effects of thermal residual stress and fibre-matrix debonding on the transverse behaviour.
3) To examine in detail the effect of thermal residual stress on the microscopic stress state under transverse shear loading. Also, to examine the effect of fibre-matrix debonding on the transverse shear behaviour of the carbon fibre/epoxy composite.

Finally, the field of multiscale modelling, and more specifically its implementation using commercial finite element codes, is receiving much attention from academic researchers (Ghosh et al. 2007), aircraft manufacturers (de Boer & Poort 2010) and commercial software developers (Firehole Technologies Inc. 2009). The development of such tools can provide widespread access to novel multiscale computational approaches and, consequently, may have some commercialisation potential. Thus, the final objective of this work may be identified as follows,

4) To develop a micromechanics analysis tool for composite materials, which provides efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. Also, demonstrate the functionality of the newly developed analysis tool using a number of illustrative case studies.

The findings of this thesis will provide novel insights into the onset and evolution of local deformation and damage mechanisms in fibre reinforced composites under a wide range of loading scenarios in the transverse plane. The findings will also facilitate a better understanding of the effect that local intra-ply properties, such as thermal residual stress, fibre-matrix debonding, local fibre volume fraction and fibre distributions, have on the macroscopic response of fibre reinforced composites.

1.4 Overview of Thesis

In Chapter 2, a literature review is presented which addresses numerous issues which affect microscopic damage evolution, with a considerable focus on local microscopic fibre distributions and their accurate description in micromechanical models. The review also details suitable techniques to effectively describe non-linear constitutive material behaviour and discrete microscale damage processes.

In Chapter 3, a combined experimental-numerical approach is presented where actual experimental distributions, measured from a high strength carbon fibre/epoxy
composite, are considered in the development of a novel method to generate statistically equivalent fibre distributions for high fibre volume fraction composites.

In Chapter 4, a micromechanics damage model is presented which collectively investigates the effects of thermal residual stress, fibre-matrix debonding and local fibre distribution on the transverse fracture behaviour of a fibre reinforced composite. The Nearest Neighbour Algorithm (NNA) (Vaughan & McCarthy 2010) which is developed in Chapter 3 is used to generate the finite element models for the analysis.

In Chapter 5, the behaviour of the carbon fibre/epoxy composite is examined under transverse shear loading. In particular, the effect of a number of intra-ply properties, such as thermal residual stress, fibre-matrix debonding and local fibre volume fraction, are considered. Also, using a combined transverse normal and shear loading regime, the effect of thermal residual stress on the transverse fracture surface is determined.

In Chapter 6, a micromechanics analysis tool for composite materials is developed using MATLAB, which provides efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. Also, a number of case studies are presented highlighting the features of the newly developed analysis tool, while also providing further insight into microscale deformation processes.

Finally, Chapter 7 provides the concluding remarks and some further discussion on the work carried out in this thesis. Also, a number of recommendations are outlined in terms of future directions of the work.
Chapter 2

Literature Review

2.1 Introduction

In this chapter, a review of the literature relevant to micromechanical modelling of damage and failure in fibre reinforced composite materials is carried out. This review addresses numerous issues which affect microscopic damage evolution, with a considerable focus on local microscopic fibre distributions and their accurate description in micromechanical models. The review also details suitable techniques to effectively describe non-linear constitutive material behaviour and discrete microscale damage processes. To provide a suitable context for much of the reviewed literature, an initial overview is provided into the microscopic damage accumulation process which is incipient to the macroscopic failure of composite laminates. Also, some of the current numerical strategies used to predict damage and failure in composite materials are outlined.

2.2 Damage and Failure in Composite Materials

This section outlines the microscopic damage mechanisms responsible for the failure of composite plies under various loading configurations. Also, it provides an overview of some current methods used in the numerical simulation of damage and failure for composite materials.
2.2.1 Damage Mechanisms in Fibre Reinforced Composites

Fibre reinforced composites exhibit a gradual damage accumulation to failure with a multitude of hierarchical dissipative mechanisms responsible for the deterioration of mechanical properties. The inhomogeneous and anisotropic nature of each individual composite ply means that failure, and the interaction of local damage mechanisms during the failure process, is highly dependent on the direction of loading. Various combinations of intra-ply failure mechanisms, including fibre-matrix debonding, matrix micro-cracking, matrix yielding, fibre buckling or fibre fracture, contribute to gradual ply degradation. Generally, the first local failures in laminate configurations are observed in transverse plies, as loading is perpendicular to the fibre direction and the ply strength is largely dominated by the matrix or fibre-matrix interface properties.

Transverse tensile loading results in failure through transverse ply cracking, which occurs perpendicular to the loading direction, as shown in Fig. 2.1 (a). Loading initially causes fibre-matrix debonding which in turn leads to matrix micro-cracking and/or matrix yielding which finally results in a transverse ply crack (Hobbiebrunken et al. 2006). Transverse compressive loading results in matrix dominated failure along a plane parallel to the fibres. Typically, a shear fracture path forms in the matrix phase inclined between 50°-56° to the through thickness direction (González & Llorca 2007a), as shown in Fig. 2.1 (b). It is not uncommon to observe some fibre-matrix debonding during the fracture process, particularly in the path of the shear band. Transverse shear loading results in a combination of fibre-matrix debonding and matrix yielding in the intra-ply region. Through the process of damage accumulation these local failures coalesce to form an interface dominated ply crack orientated at approximately 45° to the applied shear load (Hinz et al. 2009), as shown in Fig. 2.1 (c).
When loading occurs parallel to the fibre direction, the strength of the ply is generally much higher as failure is governed by the properties of the fibres. In laminate configurations, off-axis plies are likely to have undergone intense damage before failure occurs in the 0° plies, leading to a complex stress state in the laminate. For tensile loading in the fibre direction, the ply fails catastrophically through fibre fracture (and matrix failure) once the fibre failure strain is reached, as shown in Fig. 2.2 (a). Meanwhile for compressive loading in the fibre direction, ply failure is a result of fibre buckling, as shown in Fig. 2.2 (b). However, for shear loading parallel to the fibres, failure is governed by the matrix and the fibre-matrix interface and as a result the ply is much weaker. The applied load causes large shear stresses to develop in matrix regions in between fibres which eventually leads to matrix yielding and/or fibre matrix debonding, resulting in a fracture plane parallel to the fibres, as shown in Fig. 2.2 (c).
literature review

While a number of ply degradation mechanisms have been outlined, a further damage mechanism to be considered at the ‘laminate level’ is delamination or inter-ply cracking. Delamination can be caused by low velocity impact, high inter-laminar stresses (i.e. under shear loading) or the progression of intra-ply damage. This can occur for a laminate under a tensile load where transverse cracks have developed in the 90° plies. Due to the stress concentration at the crack tip, delamination between the neighbouring ply is likely to occur once the crack propagates to the ply boundary, as shown in Fig. 2.3 (a). For a laminate under a tensile load, the presence of an inter-ply crack is not detrimental as, due to the loading direction, the inter-ply crack cannot open and the laminate is dominated by the strength of the fibres, as shown in Fig. 2.3 (a). However, under a compressive load, inter-ply cracks reduce the through thickness strength and this results in buckling behaviour, as shown in Fig. 2.3 (b), which can greatly reduce the compressive strength of the laminate.
Despite the fact that failure in a composite is a consequence of damage mechanisms occurring at, or below, a microscopic level, many of the current numerical methods used to predict failure in laminated structures are based at the mesoscopic or ply level. Progressive damage analysis (PDA) is one such approach where, an initial undamaged material state is assumed and classical failure criteria, such as Hashin (1980), are employed to predict the onset of local failures at each material point in a finite element model. Once the failure criteria has been met, a damage variable is introduced which degrades the initial material stiffness of that particular material point. The softening behaviour can be represented in number of ways, such as instantaneous unloading, linear or non-linear degradation models.

While this method is termed a ‘progressive’ approach it actually ignores much of the non-linear behaviour which occurs due the onset of certain sub-critical microscopic damage mechanisms, such as matrix micro-cracking or fibre-matrix debonding, early in the loading history. This has led to the development of advanced Continuum Damage Mechanics (CDM) models which predict damage induced stiffness reduction, prior to ultimate material failure, using effective damage parameters to represent ply degradation mechanisms. In the CDM approach, it is assumed that the nucleation of micro-cracks and voids cause a reduction in the resisting area of the material, as shown in Fig. 2.4. Although these local fracture mechanisms are not modelled discretely, their effect is accounted for by introducing a generalised damage
tensor \((d_{ij})\) and defining an equivalent or homogenised material region where a new effective stress \((\overline{\sigma})\) is now acting, as shown in Fig. 2.4.

![Diagram showing homogenisation and localisation](image)

**Figure 2.4:** Concept of replacing discrete cracking process with an effective continuum.

Although these models allow for an adequate prediction of experimental non-linear behaviour, they still rely on non-physical material parameters, such as damage/plasticity coupling factors, to account for non-linear behaviour. Also, they offer little insight into the process of damage accumulation and its overall affect on the material response. Consequently, computational micromechanics has emerged as an effective technique to determine relevant interactions between constituent phases, while also allowing for the prediction of local microscale damage processes and their subsequent effect on macroscopic or structural behaviour.

### 2.3 Micromechanics

Micromechanics problems are solved using homogenisation and localisation concepts to provide a link between multiple length scales. Homogenisation may be interpreted as describing the behaviour of a microscopically heterogeneous material in terms of an equivalent homogenous reference material at the macroscopic scale. Meanwhile, localisation may be described as determining local responses in the constituent phases of the heterogeneous microstructure from applied macroscopic loading configurations. This is shown schematically in Fig. 2.5 whereby at the point \(P\), the macroscopic homogenous material can be characterised by a sample volume of the
heterogeneous microstructure. The sample volume chosen at the microscale should be sufficiently large such that a continuum approach provides an adequate description of behaviour for each constituent phase, but much smaller than the characteristic length of the macroscopic sample (Kouznetsova et al. 2001).

The field of micromechanics is extensive and a wide range of strategies are available to predict material behaviour at multiple length scales, including periodic homogenisation models, mean field methods, bounding methods or embedding approaches. Extensive reviews which outline the aforementioned methods have been carried out by Bohm (1998), Trias (2005) and Pindera et al. (2009). In the context of computational micromechanics, the method most widely used is the periodic homogenisation approach and, as a result, this section provides the theory and background on which periodic homogenisation is formulated.

2.3.1 Periodic Homogenisation Approach

For periodic homogenisation, the concept of periodicity is used to represent heterogeneous materials, where it is assumed that the macroscopic body can be composed of an infinite array of repeating unit cells (RUCs). Due to the repetitive nature of the microscopic deformation, boundary pairs of the RUC should be compatible, such that the array of RUCs should ‘fit’ together to form the macroscopic equivalent body, as
shown in Fig. 2.6. This implies that boundary pairs of the RUC, i.e. (i) **North** and **South** and (ii) **East** and **West** shown in Fig. 2.6, must undergo the identical deformations. Also, the stress should be continuous through the boundaries of the unit cell, implying that the stress vectors are equal and opposite for each boundary pair. These conditions are achieved through the application of periodic boundary conditions, which have been shown by Van der Sluis et al. (2000) and Terada et al. (2000) to give a better estimation of effective properties than either homogeneous traction or displacement boundary conditions. Periodic boundary conditions are implemented through a series of kinematic ties acting on the boundary faces, which can be expressed in terms of the nodal displacement vector, \( \mathbf{u} \), such that,

\[
\mathbf{u}_{\text{North}} - \mathbf{u}_{n_4} = \mathbf{u}_{\text{South}} - \mathbf{u}_{n_1} \tag{2.1}
\]

\[
\mathbf{u}_{\text{West}} - \mathbf{u}_{n_1} = \mathbf{u}_{\text{East}} - \mathbf{u}_{n_2} \tag{2.2}
\]

where the subscripts **North**, **South**, **East** and **West** correspond to nodes situated on each boundary of the RVE and subscripts \( n_1, n_2 \) and \( n_4 \) correspond to the control nodes which are located at each corner of the RUC, as shown in Fig. 2.6.

![Figure 2.6: Periodic boundary conditions applied to a microscopically heterogeneous material.](image)

For the macroscopic equivalent body shown in Fig. 2.6, the stress state is globally or macroscopically homogeneous over the domain, as all cells within the domain have undergone the same loading conditions (Anthoine 1995). With the application of a macroscopically homogeneous stress or displacement field on the
sample volume of the heterogeneous microstructure, homogenisation can be carried out by determining volume averages of resulting microscopic state variables. In the context of a heterogeneous composite microstructure it is desirable to determine the average stresses ($\bar{\sigma}_{ij}$) and average strains ($\bar{\varepsilon}_{ij}$) and these can be described using the following relations,

\[
\bar{\sigma}_{ij} = \frac{1}{V} \int \sigma_{ij} dV \tag{2.3}
\]
\[
\bar{\varepsilon}_{ij} = \frac{1}{V} \int \varepsilon_{ij} dV \tag{2.4}
\]

where $V$ is the sample volume of the material. The average stress and strain can be related using the effective elastic stiffness tensor, $C_{ijkl}$, and the effective compliance tensor, $S_{ijkl}$,

\[
\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \tag{2.5}
\]
\[
\varepsilon_{ij} = S_{ijkl} \sigma_{kl} \tag{2.6}
\]

In order for a suitable description of material behaviour, in both the resolution of local state variables at the microscale and also the accurate prediction of macroscopic equivalent properties, a sample volume of the material microstructure which is deemed representative of the bulk microstructure should be used. This sample volume is termed the Representative Volume Element (RVE).

### 2.3.2 Representative Volume Element

The idea of an RVE was first put forward by Hill (1963), who defined it as a region which (i) must be structurally entirely typical of the whole microstructure on average and (ii) must contain a sufficiently large number of microstructural heterogeneities for apparent overall moduli to be effectively independent of the surface values of traction and displacement (as long as these values are macroscopically uniform). Drugan & Willis (1996) define an RVE to be the smallest material volume element for which the usual spatially constant ‘overall modulus’ is a sufficiently accurate model to represent mean constitutive response.
These early definitions of the RVE led to the development of periodic fibre unit cells to represent the composite microstructure. These models assume a regular, repeating array of fibres in the microstructure. It has normally been assumed that the fibres are packed in either a square or hexagonal arrangement, as shown in Fig. 2.7. These representations have yielded accurate results in determining elastic properties when subjected to homogenous boundary conditions (Sun & Vaidya 1996) and, due to their simplicity, are computationally efficient. However, in the prediction of damage, these models assume that when damage occurs at the fibre-matrix interface (within the micromechanical model), it occurs simultaneously across every fibre-matrix interface in the microstructure. The same is true for damage occurring in regions of the matrix. This is not accurate in most cases and so failure related predictions have been poor using these simple approaches (Swamithan et al. 2006).

Figure 2.7: Regular fibre arrays and their associated periodic fibre unit cells: (a) square and (b) hexagonal periodic fibre arrays.

Figure 2.8 shows a cross-sectional view of a carbon fibre/epoxy composite, where it can be seen that the distribution of fibres is not periodic due to the existence of apparently random fibre rich and fibre denuded regions. While this does not significantly affect the macroscopic mechanical properties, these regions cause an irregular stress distribution to exist across the microstructure, particularly when loading occurs in the transverse plane, allowing microscopic damage mechanisms to occur more
easily. Pyrz (1994a) showed experimentally that the transverse failure stress of a polymer matrix composite is significantly influenced by the type of spatial pattern present. It was also shown that the nearest neighbour distances between fibres has a considerable effect on stress in the microstructure, with peak stresses occurring in regions where fibres lie in close proximity to one another. Also, Lewandowski et al. (1989) showed that for a metal matrix composite under transverse loading, locations with reinforcement clustering were more likely to suffer damage initiation and accumulation.

Using computational micromechanics, the effects of fibre distribution have been examined by Brockenbrough et al. (1991) for a metal matrix composite (MMC) reinforced with continuous fibres. It was concluded that when loading occurred in the transverse plane, the non-periodic arrangement of fibres plays a key role in the behaviour of the material and that a periodic model cannot correctly predict the transverse deformation seen in a non-periodic composite. Böhm et al. (1993) showed using a finite element micromechanical model that the fibre arrangement of a unidirectional MMC has little effect on the overall thermo-mechanical properties. However, the computed micro-fields were found to be heavily dependent on the fibre arrangement and it was concluded that damage related parameters such as interfacial stress distributions are influenced by the fibre distribution. Trias et al. (2006b) examined in detail the stress and strain distributions resulting from a transverse tensile load applied to both a random fibre array model and a periodic fibre array model of a

![Micrograph of a carbon fibre composite showing spatial arrangement of fibres.](Image)

Figure 2.8: Micrograph of a carbon fibre composite showing spatial arrangement of fibres.
carbon fibre composite. It was concluded that the use of periodic fibre unit cells could lead to an underestimation of microscale damage initiation. Hojo et al. (2009) used a micromechanical model to investigate the effect of local fibre distribution on the interfacial stress state for a unidirectional carbon fibre epoxy laminate loaded in transverse tension. It was found that for an irregular fibre array the absolute value of the Interfacial Normal Stresses (INS) rapidly increased when the distance between neighbouring fibres was less than 0.5µm and when they were aligned with the loading direction. It was also found that a periodic hexagonal model under the same loading conditions could not represent the microscopic stress state.

In order to model the onset and evolution of microscopic damage accurately the non-uniform spatial arrangement of fibres needs to be captured. This means that the microstructure of the composite needs to be represented in an ‘equivalent’ sense, meaning that not only should an RVE exhibit the same elastic behaviour as the bulk material, as stipulated in early definitions (Hill 1963), but it should also capture the overall characteristics of the fibre arrangement within the microstructure. This has led to the definition of a Statistically Equivalent RVE which, according to Swaminathan et al. (2006), is the smallest region of the microstructure which satisfies the following criteria,

i. Its effective stress-strain behaviour should be equivalent to the overall behaviour of the material.
ii. The distribution functions of parameters reflecting the local morphology should be equivalent to those for the overall microstructure.
iii. It should be independent of location in the local microstructure and the applied loading conditions.

2.4 Analysis of Fibre Distributions in Composite Microstructures

Determining a suitable RVE which has equivalent morphological characteristics as the microstructure at large relies on the fibre distribution within the microstructure being sufficiently characterised. This is generally carried out using spatial point pattern analysis. This section outlines a number of statistical descriptors which fully characterise the spatial arrangement of fibres in the microstructure. Also, a number of
numerical and experimental strategies which have been used to generate fibre distributions are reviewed.

2.4.1 Spatial Point Patterns

Spatial point pattern analysis uses distance based techniques to analyse the arrangement of a set of points. Many statistical descriptors exist which characterise spatial point patterns (Diggle 2003) and these have been widely used (Bulsara et al. 1999, Buryachenko et al. 2003, Trias et al. 2007, Melro et al. 2008) to characterise the microstructural arrangement in composite materials by considering the positions of all fibre centres as a spatial point pattern. The most fundamental type of spatial point pattern is known as a random point field, which is shown in Fig. 2.9 (a), and many of the methodologies used to generate non-uniform fibre distributions are derived from this type of point pattern (Buryachenko et al. 2003). A random point field is a field whose points are chosen on a uniform random basis such that the location of any point is completely independent of the locations of all other points in the field. This means that the probability of a point lying within any infinitesimal region should be the same in any region of the field. This type of field is said to exhibit Complete Spatial Randomness (CSR). However, the microstructure of the composite under investigation consists of fibres that are of non-zero size and cannot be considered as points. As a result, this CSR pattern commonly serves as a comparison for other spatial point patterns (Pyrz 1994b, Trias 2005). Spatial point patterns can exhibit various other distributions such as a regular, dispersed or clustered arrangements of points, as shown in Figs. 2.9 (b), (c) and (d), respectively.
Nearest Neighbour Distribution Functions

Nearest neighbour distribution functions detail the short range interaction of fibres by analysing the distance between each fibre and their $n^{th}$ closest neighbour.
(Diggle 2003). For example, the 1st nearest neighbour distribution function is found by calculating the distance from each fibre to their closest neighbouring fibre. Similarly, the 2nd nearest neighbour distribution function can be found by calculating the distance from each fibre to their 2nd closest neighbour.

**Second-Order Intensity Function**

The second-order intensity function, also known as Ripley’s $K$-function, has been widely used to distinguish between different types of point patterns (Pyrz 1994b, Trias 2005). The function, $K(r)$, is defined as the number of further points expected to lie within a radial distance, $r$, of an arbitrary point, as shown in Fig. 2.10, divided by the number of points per unit area. The boundary of the domain has a significant effect when calculating this function and an estimator which accounts for edge-correction has been established by Ripley (1977),

$$K(r) = \frac{A}{N^2} \sum_{k=1}^{N} w_k^2 I_k(r)$$

(2.7)

where $N$ is the total number of points in the area, $A$. $I_k(r)$ is the number of points lying within a radial distance, $r$, of a given fibre and $w_k$ is the ratio of the circumference lying within the area, $A$, to the whole circumference of the circle.

![Figure 2.10: Radial area of influence for calculating the second-order intensity function and radial distribution function.](image)
The $K$-function can distinguish characteristics present in point distributions, such as short range regularity or long range clustering. Generally, point fields are compared against a pattern exhibiting complete spatial randomness, for which the $K$-function of the domain can be analytically evaluated as,

$$K(r) = \pi r^2$$  \hspace{1cm} (2.8)

For clustered distributions $K(r)$ will lie above the CSR pattern and will tend to diverge away from it at larger distances, as clustering becomes more prominent. When $K(r)$ lies below the CSR pattern, the distribution is likely to show some level of regularity. Periodic arrangements exhibit a stair shaped function due to the equal spaces between inclusions.

**Radial Distribution Function**

The radial distribution function describes how the average fibre density varies as a function of distance from a given fibre centre. It is found by determining the number of fibres lying within an annular region of inner radius, $r$, and outer radius, $r+dr$, as shown in Fig. 2.10, and dividing this by the average number of fibres per unit area. It is closely related to the derivative of the second order intensity function and is mathematically defined as,

$$G(r) = \frac{1}{N_a(2\pi r)} \frac{dK(r)}{dr}$$  \hspace{1cm} (2.9)

where, $dK(r)$ is the average number of fibre centres lying within an annulus of inner radius, $r$, and outer radius, $r+dr$, and $N_a$ is the number of fibres per unit area (Yang et al. 1997). Although related to the second order intensity function, the radial distribution function provides quite different quantitative information regarding the average fibre density at a radial distance, $r$, from a given fibre. It identifies most frequent distances between points signified by local maxima and least frequent distances between points signified by local minima. The radial distribution function for a CSR pattern is unity for all distances, indicating that points have no tendencies to either cluster or observe regular arrangements. For any statistically homogenous point pattern the value of $G(r)$ approaches 1 for large values of $r$, as the area of the circular annulus becomes large enough to be representative of the average fibre density of the overall region.
2.4.2 Numerical Algorithms developed for Microstructure Generation

The hard core random field has been widely used to represent the non-uniform arrangement of fibres in a composite microstructure. The hard-core random field is an extension of the random point field, described earlier, however it includes a condition accounting for the physical areas taken up by the fibres (Ohser 2006). The model essentially represents the fibres as a set of non-overlapping disks, whose centres have been randomly distributed inside the domain. This means that the probability of finding a fibre centre within another fibre is zero and is non-zero for regions outside the fibre boundary. Random Sequential Adsorption (RSA) is commonly used to generate the hard-core random field. The simulation process sequentially places fibres in random positions within the domain. If a newly deposited fibre overlaps with any pre-existing fibre, it is rejected and a new random centre position is generated. Once the fibre does not overlap with any pre-existing fibres, its position is fixed and does not move. The process is repeated until desired fibre volume fraction is achieved. Yang et al. (1997) used the hard-core model effectively to generate a non-uniform spatial arrangement of fibres in a ceramic matrix composite, with a fibre volume fraction of 35%. First and second nearest neighbour distribution functions were used to verify that the resulting distributions were equivalent to the real composite microstructure which was experimentally characterised using digital image analysis.

However, one of the constraints of the hard-core model is that it is subject to a jamming limit, which means it does not permit fibre volume fractions greater than ~54% being generated (Hinrichensen et al. 1986). Therefore, it cannot be used to represent the microstructures of high strength composite materials which generally have fibre volume fractions in excess of this. To overcome this intrinsic characteristic of the hard-core model, Melro et al. (2008) used an initial configuration generated by the hard-core model followed by a fibre stirring algorithm to create matrix rich regions in the RVE, allowing more fibres to be allocated positions. The stirring procedure is carried out for each fibre in the region and causes fibres to move towards neighbouring fibres by small random displacements. This process is shown in Fig. 2.11, where the fibre A is displaced towards its neighbouring fibre B, by a random displacement, M1, to take new position, A1. The fibre now undergoes another random displacement, M2, in the direction of its 2nd nearest neighbour C to take up a new position A2. Further iterations
are carried out where the fibre is displaced in the direction of neighbouring fibres as before. This method is successful in unlocking the hard-core model from its jamming configuration and it can achieve fibre volume fractions of 65%. The resulting fibre arrangements were analysed using first and second nearest neighbour distributions, radial distribution functions and second order intensity functions to show the arrangement could be described by a random distribution.

Wongsto & Li (2005) used an initial periodic hexagonal fibre array of the desired volume fraction and created a non-uniform fibre distribution using a fibre shaking algorithm. This forces a given fibre to undergo an arbitrary displacement in a randomly chosen direction such that the relocation does not cause an overlap with any neighbouring fibres. This process is repeated for each fibre in the domain and results in a non-uniform distribution of fibres. However, the resulting distributions have not been statistically analysed and so the exact type of pattern which results is not clear. Qing & Mishnaevsky Jr (2009) used a similar approach, however, due to the very high fibre volume fractions used, which were in the region of 65-85%, the distributions generated fail to depart greatly from their initial regular arrangement. Trias (2005) also used a similar fibre shaking approach based on the random close packing of spheres (Berryman 1983). Firstly, the number of fibres needed to achieve the required fibre volume fraction is determined. These fibres are then randomly distributed within a square
domain which results in a large number of fibres overlapping with one another. The fibre shaking algorithm then applies a number of random displacements to any overlapping fibres, iterating until all fibres within the domain are independent of one another. While this approach is successful in achieving a fibre volume fraction of 60%, due the large amount of computational time required to achieve such fibre volume fractions (which was in excess of 120mins) it was concluded that this method was impractical.

2.4.3 Experimental Microstructure Patterns

Many of the preceding numerical approaches assume that the microstructure of a composite material is characterised by a random distribution of fibres. However, the spatial arrangement of fibres in a composite microstructure is not necessarily described by a random distribution. Their arrangement can vary significantly depending on a number of factors. Pyrz (1994b) showed that for three different curing conditions applied to a glass fibre/epoxy composite, the resulting spatial patterns in each microstructure were affected. Using the second-order intensity function, the spatial patterns were analysed and were each found to differ considerably and also not conform to a CSR pattern, as shown in Fig. 2.12. It was concluded that the spatial pattern of the microstructure was neither regular nor random, and is highly dependent on the manufacturing and processing conditions. It was also shown for the materials analysed that their probability density functions of nearest neighbour distances do not follow the same form as those of a CSR pattern.

![Figure 2.12: Second order intensity function showing varying fibre patterns (reproduced from Pyrz (1994b)).](image-url)
Trias (2005) analysed the microstructures from four carbon fibre composites and found that the fibre distribution for three of these materials departed from a CSR pattern, each showing distinctive statistical distributions. It was concluded that because of the possible variance of statistical distributions from one composite material to another, a microstructure reproduction approach is more appropriate for micromechanical modelling than the use of specific algorithms which are only capable of reproducing fibre distributions conforming to a CSR pattern. Trias et al. (2006a) and Grufman & Ellyin (2008) have used a direct microstructure reproduction methodology to convert an observed microstructure of a studied material to a finite element model, as shown in Fig. 2.13, through the use of digital image analysis techniques.

![Figure 2.13: Direct microstructure approach (from Trias (2005)).](image)

However, unlike most numerical approaches, representative microstructure images are not strictly periodic, such as the image shown in Fig. 2.13. This presents difficulties when periodic boundary conditions are to be applied and as a result alternative methods such as the embedded cell approach must be employed to ensure macroscopically uniform loading. Bulsara et al. (1999) also highlighted direct microstructure reproduction as an impractical method to generate micromechanical models as it is not known, in terms of damage initiation, which areas of the microstructure will be of interest and analysing one part of the microstructure could give significantly different results to another area. This is illustrated by Silberschmidt (2008) who showed that convergence of the fibre volume fraction parameter for different window sizes of the microstructure is relatively slow, as shown in Figs. 2.14 (a) and (b). Here, different locations in the microstructure were analysed, as shown in Fig. 2.14 (a), and the mean values of volume fraction, as well as maximum and minimum values, were plotted for different window sizes, as shown in Fig. 2.14 (b). This
implies that a large RVE size is needed to incorporate the statistical distribution of fibres. Numerical algorithms, which are generally based on generating a distinct fibre volume fraction, are possibly at an advantage in terms of minimum size of the RVE as the fibre volume fraction for all sizes generated should be within the bounds of the RVE definition.

![Image](image.jpg)

Figure 2.14: (a) Variation of local fibre volume fraction (from Silberschmidt (2008)) and (b) Convergence of local fibre volume fraction with window size (reproduced from Silberschmidt (2008)).

### 2.4.4 Optimum size of the Representative Volume Element

As already outlined, the early definitions of the RVE put forward by Hill (1963) and Drugan & Willis (1996) led to the development of periodic fibre unit cells, from which accurate predictions of overall moduli could be obtained (Sun & Vaidya 1996). However, the contribution of the microscopic stress/strain fields on the failure process has been well established and has meant recent definitions of the RVE, such as those by Swaminathan et al. (2006) or Grufman & Ellyin (2008), require correlation of statistical distributions describing the fibre arrangement, allowing an accurate representation of damage behaviour. The size of the RVE can be represented by the variable $\delta$, which relates length of the side of the RVE, $L$, to the fibre radius, $r_f$, using the following simple relationship,

$$\delta = \frac{L}{r_f} \quad (2.10)$$

A wide range of studies have been carried out examining RVE size and these have yielded contrasting results. Shan & Gokhale (2002) characterised the geometrical
arrangement of a ceramic matrix composite microstructure having a fibre volume fraction of 35% using image analysis techniques. By analysing the nearest neighbour distribution functions for different sized microstructural windows along with FE simulations, it was determined that the optimum RVE size was $\delta \approx 40$. Trias et al. (2006c) determine that for a typical carbon fibre reinforced plastic, having a fibre volume fraction of 50%, the optimum size of the RVE was $\delta = 50$. The mechanical and statistical criteria considered for the analysis were the effective properties, the mean and variance of stress and strain fields, probability density functions of the stress and strain components in the matrix and nearest neighbour distributions. González & Llorca (2007a) showed for a carbon fibre/epoxy composite having a fibre volume fraction of 50% an RVE containing 30 fibres ($\delta = 12$) was sufficient to predict the macroscopic response. This was verified by considering the averaged response of a number RVEs containing 30 fibres compared to an RVE containing 70 fibres where a reasonably small variance was found between resulting stress-strain curves for both sized RVEs.

2.5 Effect of the Constituent Materials on Mechanical Behaviour

The transverse tensile response of both a carbon fibre/epoxy composite (HTA/6376) and a glass fibre/epoxy (S2/FM94) composite are shown in Fig. 2.15. The response of the glass fibre/epoxy composite is highly non-linear which is markedly different to the largely linear response to failure of the carbon fibre/epoxy composite (O’Higgins et al. 2009). Obviously, the different responses are a direct result of the properties of the microstructure and the configuration of the constituent phases, i.e. fibre volume fraction, matrix yield strength, fibre-matrix interface strength/toughness and thermal residual stress. This section outlines a number of pertinent issues associated with the mechanical behaviour of epoxy matrices, the fibre-matrix interface properties and the presence of thermal residual stress.
yielding on the hydrostatic component of the applied stress state. Between tensile and compressive yield strengths suitable to predict yielding in polymers. As a result, Mises, are not influenced by the hydrostatic component of stress and as a result are not behaviour under tensile, compressive and shear loading and this is attributed to the role characteristics. They generally have superior mechanical properties post-cure, exhibit low shrinkage during curing and offer good resistance to moisture effects.

Epoxies are a group of thermosetting polymers formed from the reaction of an epoxide resin and a polyamine hardener during the curing process. The use of epoxy matrices in fibre reinforced composites offer distinct advantages over alternatives, such as polyester or vinyl ester resins, as they exhibit superior adhesion qualities which ensure homogenous bonding to fibres, allowing for excellent load transfer characteristics. They generally have superior mechanical properties post-cure, exhibit low shrinkage during curing and offer good resistance to moisture effects.

The behaviour of epoxy resins has been shown to be dependant on the applied stress state. Fiedler et al. (2001a) showed that they exhibit different deformation behaviour under tensile, compressive and shear loading and this is attributed to the role of the hydrostatic stress on the yielding behaviour. Classic failure criteria, such as Von-Mises, are not influenced by the hydrostatic component of stress and as a result are not suitable to predict yielding in polymers. As a result, Raghava et al. (1973) proposed a modified pressure dependant Von-Mises criteria which accommodates for the difference between tensile and compressive yield strengths and accounts for the dependence of yielding on the hydrostatic component of the applied stress state. In its general form the modified Von-Mises criteria may be expressed as,

\[
\text{F} = \sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2 - 3\tau_1^2}
\]

Figure 2.15: Transverse tensile response of carbon fibre/epoxy and glass fibre/epoxy composites (from O'Higgins et al. (2009)).

2.5.1 Epoxy Matrix Behaviour

Epoxies are a group of thermosetting polymers formed from the reaction of an epoxide resin and a polyamine hardener during the curing process. The use of epoxy matrices in fibre reinforced composites offer distinct advantages over alternatives, such as polyester or vinyl ester resins, as they exhibit superior adhesion qualities which ensure homogenous bonding to fibres, allowing for excellent load transfer characteristics. They generally have superior mechanical properties post-cure, exhibit low shrinkage during curing and offer good resistance to moisture effects.
\[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 + 2(\sigma_T - \sigma_T)(\sigma_1 + \sigma_2 + \sigma_3) = 2\sigma_T \sigma_C \] (2.11)

where \(\sigma_1\), \(\sigma_2\) and \(\sigma_3\) are the principal stresses and \(\sigma_T\) and \(\sigma_C\) are the tensile and compressive strengths of the material, respectively. In this expression, the dependence of the yielding behaviour on the hydrostatic stress is introduced by the term \((\sigma_1 + \sigma_2 + \sigma_3)\), which is the first invariant of the stress tensor. It should be noted that if the tensile and compressive strengths are equal, i.e. \(\sigma_T = \sigma_C\), the expression reduces to the classical form of the Von-Mises criterion.

More recently, Asp et al. (1996a) proposed the dilatational energy density criterion for matrix initiated failure. The criterion assumes that failure occurs when the dilatational energy density \(U_v\) reaches a critical value. It is formulated as a function of the principal stresses \((\sigma_1, \sigma_2, \sigma_3)\) and is given by the following equation,

\[U_v = \frac{1 - 2\nu}{6E} (\sigma_1 + \sigma_2 + \sigma_3)\] (2.12)

where \(E\) and \(\nu\) are the Young’s modulus and Poisson’s ratio, respectively. The criterion has been used in a number of studies (Asp et al. 1996b, Fiedler et al. 2001b, Trias et al. 2006a) to predict matrix initiated failure under transverse tensile loading.

The Mohr-Coulomb criterion has also been widely used to predict failure in polymers. The Mohr-Coulomb criterion states that yielding will occur when, for a given plane, the shear stress \(\tau\) and the normal stress \(\sigma_n\) reach a critical combination such that,

\[\tau = c - \sigma_n \tan \phi\] (2.13)

where \(c\) is the cohesion yield stress and \(\phi\) is the angle of internal friction. In physical terms the cohesion \(c\) (initial cohesion stress) is the yield stress under pure shear and the friction angle accounts for the effect of hydrostatic stress. The yield locus of the Mohr-Coulomb criterion can be visualised in the Mohr stress space, as shown in Fig. 2.16. Here, the elastic domain of the Mohr-Coulomb law is the set of stresses where all three Mohr circles are below the yield locus which is defined by Equation 2.13, as shown in Fig. 2.16.
From Fig. 2.16, the Mohr-Coulomb yield condition (Equation 2.13) may be expressed in terms of the maximum and minimum principal stresses by the following equation,

$$(\sigma_1 - \sigma_3)\cos\phi = c - \left(\frac{\sigma_1 + \sigma_3}{2}\right) + \frac{\sigma_1 - \sigma_3}{2}\sin\phi \tan\phi$$

(2.14)

where $\sigma_1$ and $\sigma_3$ are the maximum and minimum principal stresses, respectively. By rearranging Equation 2.14, a yield function, expressed in terms of the maximum and minimum principal stresses, may be defined as follows,

$$f(\sigma_1, \sigma_3) = (\sigma_1 - \sigma_3) + (\sigma_1 + \sigma_3)\sin\phi - 2c\cos\phi$$

(2.15)

The corresponding yield surface of the Mohr-Coulomb criterion may be visualised in the principal stress space as a hexagonal pyramid, aligned with the hydrostatic axis (i.e. $\sigma_1 = \sigma_2 = \sigma_3$), whose apex is located on the tensile side of the hydrostatic axis, as shown in Fig 2.17 (a). The pyramidal shape of the Mohr-Coulomb yield surface is a result of the pressure sensitivity of the criterion which predicts the asymmetry between the tensile and compressive strengths of the material. This is in contrast to the Von-Mises criterion whose cylindrical yield surface, shown in Fig. 2.17 (b), predicts the same strength in tension and compression. It should be noted that the friction angle controls the shape of the yield surface. The range of values the friction angle can assume is $0^\circ > \phi > 90^\circ$, where in the absence of internal friction (i.e. for $\phi = 0^\circ$), the surface will reduce to the prismatic hexagonal Tresca surface. Meanwhile, for $\phi = 90^\circ$ the surface reduces to the Rankine model which has a triangular deviatoric section.
Meanwhile, the Drucker-Prager has been proposed as a smooth approximation to the Mohr-Coulomb law. It is formulated based on the Von-Mises criterion but, like the Mohr-Coulomb law, includes an extra term to account for pressure sensitivity. The Drucker-Prager criterion states that plastic yielding begins when the $J_2$ invariant of the deviatoric stress and the hydrostatic stress, $p$, reach a critical combination. The criterion may be expressed as follows,

$$\sqrt{J_2 + \eta p} = \bar{c}$$

(2.16)

where $\eta$ and $\bar{c}$ are functions of the internal friction angle, $\phi$, and cohesion stress, $c$, respectively. In the principal stress space, the Drucker-Prager criterion may be
visualised by a circular cone, whose apex is aligned with the hydrostatic axis, as shown in Fig. 2.17 (c). It is common to approximate the Drucker-Prager yield surface based on the Mohr-Coulomb description of material behaviour (i.e. in terms of the cohesion stress, $c$, and internal friction angle, $\phi$), which means that the Drucker-Prager cone becomes coincident with the edges of the Mohr-Coulomb pyramid. Due to the continuous nature of the Drucker-Prager yield surface, it allows for easier computational implementation.

While both the Mohr-Coulomb and Drucker-Prager criteria exhibit similar characteristics, the Mohr-Coulomb criterion has already been widely used to predict the onset of yielding in polymers, particularly those associated with fibre reinforced composite materials. Experimental investigations have shown that the Mohr-Coulomb assumption of a linear dependence of the yield stress on the hydrostatic pressure provides a good description of polymer behaviour, particularly at low pressures (Altenbach & Tushtev 2001). Vural & Ravichandran (2004) suggest the Mohr-Coulomb criteria to be suitable to predict failure of glass fibre/epoxy composites due to its accurate prediction of the orientation of the shear bands under transverse compressive loading. In micromechanics simulations, the Mohr-Coulomb model has been shown to provide a good description of epoxy behaviour under transverse compressive loading (González & Llorca 2007a). It has also been used to model the behaviour of the epoxy in micromechanical simulations of fibre reinforced composites under transverse shear (Totry et al. 2008a), transverse tensile (Zhang 2010) and combined loading scenarios (Totry et al. 2008a, c).

2.5.2 Fibre-Matrix Interface

A typical composite material consists of two discrete phases, i.e. the fibre and the matrix. The layer/boundary where the two phases meet is called the ‘interface’ while the region adjoining the interface is known as the ‘interphase’. The interphase is formed as a result of bonding and reactions between the fibre and the matrix and it is where the mechanical and physical properties change from the bulk properties of the matrix to the bulk properties of the fibre (or vice versa). In terms of volume fraction the interphase region is an insignificant portion of the overall material, however, it is the region through which the load transfer and stress redistribution from the matrix to the
fibres takes place and its influence on the overall material properties is considerable (Kim & Mai 1998).

The level of adhesion (between the fibre and the matrix) at the interface, or in other terms the interfacial strength, determines its ability to transfer load effectively. It is widely accepted that the transverse strength of a composite is largely governed by the interfacial strength (Gamstedt & Sjögren 1999). The loss of adhesion between the fibre and the matrix, also known as interfacial cracking or fibre-matrix debonding, has been examined in a number of studies in the transverse regime (Harrison & Bader 1983, Gamstedt & Sjögren 1999, Hobbiebrunken et al. 2006). Hobbiebrunken et al. (2006) carried out a combined experimental and numerical study to examine initial failure of two transversely loaded carbon fibre/epoxy composites, one which had stronger fibre-matrix interface than the other. From in-situ SEM experiments it was observed that interfacial failure initiates the transverse fracture process. For the composite with a strong interface, transverse fracture was initiated by a small number of isolated interfacial cracks occurring between neighbouring fibres with an inter-fibre distance of 0.5-1µm whose alignment was parallel with the loading direction, as shown in Fig. 2.18 (a). This was almost immediately followed by sudden failure of the ply. For the composite with a weaker fibre-matrix interface, damage initiated through widespread fibre-matrix debonding. As these interfacial debonds grow, small resin bridges formed between them which underwent significant plastic deformation until their failure, causing final fracture of the ply, as shown in Fig. 2.18 (b).
Gamstedt & Sjögren (1999) examined the onset of damage in laminates containing transverse plies and found that, for both monotonic and fatigue loading conditions, the governing micro-mechanism which leads to transverse cracking and subsequent global failure of a typical composite structure was fibre-matrix debonding. Using in-situ microscopy at the edge of the transverse ply during a traction load, it was determined that the first damage mechanism to develop was debonding between the fibre and the matrix, as shown in Fig. 2.19 (a). The onset of debonding occurred at small loads and was widespread in the transverse ply. Upon further loading a number of these interfacial cracks coalesced to form a transverse crack as shown in Fig. 2.19 (b). The development of these transverse cracks appeared to occur stochastically at different locations. This same sequence of damage development in carbon-fibre reinforced plastics for both monotonic and cyclic loading was observed in an earlier study by Harrison & Bader (1983).
Literature Review

Hinz et al. (2009) also used in-situ SEM experiments to examine the microscopic development of failure in a cross-ply fibre metal laminate subject to interlaminar shear load which was applied using the Double Notch Shear (DNS) test. It was found that intra-ply damage initiated in the transverse plies through a combination of fibre-matrix debonding, plastic deformation and micro-cracking in the matrix. Fibre-matrix debonding was found to initiate in the intra-ply region between closely neighbouring fibres which were orientated at 45° to the horizontal loading axis, as shown in Fig. 2.20. While at the ply boundary, significant shear deformation was found to occur as a result of the reduced local fibre volume fraction in this resin rich region. Here, intense local shear yielding occurred which lead to the formation of matrix micro-cracks and voids. Significantly, it was observed that delamination, or interlaminar shear failure, was caused by the coalescence of these intra-ply damage mechanisms, with fibre-matrix debonding cited as being one of the primary damage mechanisms observed.

Figure 2.19: (a) Initiation of debond in a cross-ply laminate subject to transverse loading (b) Coalescence of interface cracks to form transverse crack.

Figure 2.20: In-Situ SEM observation of fibre-matrix debonding due a transverse shear load applied during a double notch shear test.
Due to the embryonic role fibre-matrix debonding plays in the damage accumulation process of a laminate, particularly under transverse loading, any improvement to the properties at the fibre-matrix interface should improve laminate behaviour accordingly. The level of adhesion between the fibre and the matrix is largely determined by the resin formulation however, in an attempt to improve properties at the interface, fibre surface treatments, such as the application of coupling agents or silane coatings, have proven to be an effective method to increase adhesion, effectively delaying the onset of fibre-matrix debonding. Berglund and co-workers (Varna et al. 1997, Zhang et al. 1997) use a single fragmented glass fibre embedded in an epoxy to analyse the effect of a coupling agent on the Mode I fracture behaviour of the fibre-matrix interface. It was estimated that in the absence of a coupling agent the interfacial toughness was $\Gamma = 2$ J/m$^2$ and the onset of debonding occurred at an applied stress of 40 MPa. Meanwhile, with the addition of a coupling agent, the interfacial toughness was $\Gamma = 10$ J/m$^2$ (a five fold increase) and the onset of debonding occurred for an applied stress of 75 MPa. Similar toughness values for Mode I type failure have also been reported by Caimmi & Pavan (2009) and Koyanagi et al. (2009).

2.5.3 Thermal Residual Stress

The micromechanical behaviour of composite materials is further complicated by the presence of thermal residual stress which forms during the manufacturing process. Due to the mismatch in thermal expansion coefficients of the constituent phases, thermal residual stresses develop at the fibre-matrix interface during the thermal cool-down from cure temperature. Thermally induced stresses can be significant enough to cause damage to initiate in composite laminates prior to any mechanical load being applied, depending on the constituent material properties. Gentz et al. (2004) observed damage in a graphite fibre/epoxy composite due to thermal residual stress in post-cure specimens. It was found that damage occurred at the fibre-matrix interface where, in some local matrix rich regions, the matrix had pulled away from the fibre towards the resin concentration, as shown by the Point A in Fig. 2.21.
Ding & Bowen (2002) showed using a hexagonal periodic fibre unit cell that thermal residual stresses caused by the curing cycle of a metal matrix composite actually had beneficial effects on the transverse strength. During the cooling process the matrix experiences a greater thermal strain than the fibre and, as a result, large normal compressive stresses were induced at the fibre-matrix interface which must subsequently be overcome upon mechanical loading before debonding may occur. Hojo et al. (2009) showed, using a non-uniform fibre RVE, that the presence of thermal residual stress is greatly affected by the local fibre distribution and it significantly alters the microscopic stress state upon subsequent mechanical loading. It was shown that the magnitude of the thermal residual normal compressive stress at the fibre-matrix interface increased as the inter-fibre spacing decreased. It was also found that the presence of thermal residual stress greatly reduced the maximum interfacial normal stress upon subsequent mechanical loading. Also, the location of the maximum interfacial normal stress was no longer between fibres which had the shortest interfibre distance but was now between fibres which were slightly further apart, i.e. 0.5-1µm. Hobbiebrunken et al. (2008) examined the microscopic stress state and initial failure of a thermally and transversely loaded carbon fibre/epoxy composite. Interestingly, it was found that the thermal residual stress had the effect of lowering the maximum interfacial normal stress on a transversely loaded composite for all fibre arrangements, while the interfacial shear stress was largely unaffected by the presence of thermal residual stress. Meanwhile, Asp et al. (1996b) showed that the presence of thermal residual stress actually reduces the strength of transversely loaded composites when matrix-initiated failure (not interfacial) was assumed. This observation is a result of the chosen dilatational energy density failure criteria, which is a function of the hydrostatic stress.
Zhao et al. (2006) showed that the presence of residual stresses can change the location of damage initiation and subsequent evolution in transversely loaded polymer matrix composites. It was also shown that thermal residual stress can have a significant effect on the failure envelopes of composites, as shown by the envelopes generated under biaxial transverse normal loading and combined transverse and shear loading in Figs. 2.22 (a) and (b), respectively. It was found that under tension dominated loading thermal residual stress had beneficial effects whereas for shear or compression dominated loading its presence caused negative effects.

Figure 2.22: Effect of thermal residual stress on fracture surface (a) biaxial transverse normal loading and (b) transverse normal/shear loading.

### 2.6 Micromechanics Damage Models

For accurate prediction of damage using computational micromechanics, the model needs to incorporate statistically representative fibre distributions, non-linear behaviour of the matrix, interfacial decohesion and effects of thermal residual stress. Early predictions of damage and failure using micromechanics used linear elastic analysis to predict, what in most cases represented, the onset of damage based on the local microscopic stress state in either periodic fibre unit cells (Asp 1996b) or non-uniform fibre RVES (Trias 2005). In recent years, the development of user-defined material subroutines, coupled with the ease of implementation of advanced damage/fracture models in commercial finite element codes means the evolution of damage through the microstructure can be predicted. Ever increasing computational power also means multi-fibre micromechanical models can be analysed enabling more
accurate predictions of multiple microscopic damage mechanisms, such as fibre-matrix debonding, matrix micro-cracking and matrix plasticity. This section details the micromechanics damage models which have previously been proposed, together with their findings on how microscale properties affect macroscopic material behaviour.

Zhao et al. (2006) examined the initiation and evolution of matrix micro-cracking in a periodic fibre unit cell (square array) using a non-selective stiffness degradation scheme. This was implemented using a user-defined material (UMAT) subroutine in ABAQUS. For each increment, the stiffness degradation scheme monitors the stress state at each material integration point. Should the current stress state cause the failure criterion to reach its critical condition, which for this model was predicted by the max stress criterion, damage was simulated by reducing the material stiffness to 1% of the original value at that integration point. Maligno et al. (2009) used a similar approach to model matrix micro-cracking and extended it to predict interface cracking (Maligno et al. 2010). It was shown that increasing the fibre-matrix interface strength improved the ultimate strength of the composite under transverse tensile loading. If the interface strength was less than the tensile strength of the matrix, it was found that failure initiated in the interphase region whereas, if the interface strength exceeded that of the tensile strength of the matrix, failure initiated in the matrix region.

Although Maligno et al. (2010) examined the effect of interphase properties using a stiffness degradation scheme, a more widely accepted method to predict the effects of interface cracking is through the use of a Cohesive Zone Model (CZM). The CZM is implemented using special purpose cohesive elements, available in many commercial FE codes such as ABAQUS, which introduce a displacement discontinuity at the fibre-matrix interface when the local stress satisfies a critical condition. Their constitutive response is generally defined in terms of a bi-linear traction-separation law which relates the separation displacement between the top and bottom faces of the element to the traction vector acting upon it. As shown in Fig. 2.23, following the initial linear response, failure of the interface initiates when either the normal stress ($t_n$) or the shear stress ($t_s$) exceed the pre-defined normal ($t'_n$) or shear ($t'_s$) strengths. The evolution of damage at the interface is controlled by a linear softening curve meaning that once the failure stress is exceeded, the element stiffness reduces linearly until
complete failure at a specified normal ($\delta_n^f$) or shear ($\delta_s^f$) displacement. This effective displacement at failure ($\delta^f$) determines the rate of damage in the element and this is generally defined in terms of the fracture energy, $\Gamma$, which corresponds to the area under the traction separation curve. The CZM has been shown to reproduce decohesion patterns consistent with experimental observations of both fibre (Cid Alfaro et al. 2010) and particle (Segurado & Llorca 2006) reinforced composites.

Romanowicz (2009) used a CZM to examine the effect of interfacial debonding in a hexagonal periodic fibre unit cell under transverse tensile loading conditions. The interphase region was regarded as a discrete inhomogeneous region, where the properties varied radially between those of the fibre and those of the matrix. It was shown that the fibre-matrix interface strength controlled the transverse strength of the material. Ghosh et al. (2000) used a CZM to analyse the effect of interfacial debonding in a multiple fibre model which had a fibre volume fraction of 20% under transverse tensile loading. It was found that debonding initiated in fibres which were close to one another and evolved with increased straining. Kushch et al. (2010) implemented a cohesive zone model to predict fibre-matrix debonding in single, double and random multi-fibre RVEs under transverse tensile loading. The fibre-matrix interface parameters used by Kushch et al. (2010) are those which were experimentally determined by Varna et al. (1997) (discussed in Section 2.5.2). It was shown that the developed model predicted effects such as crack shielding, stress relaxation in neighbouring interfaces and macroscopic stiffness reduction due to debonded interfaces. The crack clusters
which formed in the random multi-fibre RVE also showed good agreement with the experimental observations of Gamstedt & Sjögren (1999).

The above micromechanics damage models (Ghosh et al. 2000, Romanowicz 2009, Kushch et al. 2010) assume the matrix behaved as a linear elastic material and did not consider non-linear effects, such as matrix micro-cracking or matrix plasticity. Cid Alfaro et al. (2010) developed a micromechanics damage model to examine the discrete fracture processes of both fibre-matrix debonding and matrix micro-cracking in a glass fibre/epoxy composite under transverse tensile loading. This was carried out by introducing interface elements at both the fibre-matrix interface to predict fibre-matrix debonding and also between the individual continuum elements of the epoxy to predict matrix cracking, as shown in Fig. 2.24. The behaviour of the interface elements was governed by a standard bi-linear traction-separation law and the microscale fracture patterns obtained for transverse tensile loading were characterised by numerous events of crack coalescence and bifurcation. The fracture patterns showed good agreement, in qualitative terms, with experimental observations by Gamstedt & Sjögren (1999) and Hobbiebrunken et al. (2006). It was found that the type of fracture patterns obtained depended upon the relative strength of the fibre-matrix interface and epoxy matrix. As Maligno et al. (2010) also found, if the fibre-matrix interface was weaker than the epoxy matrix, the failure pattern was a combination of fibre-matrix debonding and matrix cracking. Otherwise, if the fibre-matrix interface was stronger than the epoxy matrix, failure was characterised by matrix cracking alone.

Figure 2.24: Finite element discretisation where interface elements are located at the fibre-epoxy interface and between continuum elements in the epoxy (from Cid Alfaro et al. (2010)).

While the assumption of a linear elastic matrix prior to the onset of cracking could be seen as a reasonable assumption for the transverse tensile case (Asp et al. 2010).
1996b), the behaviour of many fibre/epoxy composites under shear dominated loading can be highly non-linear, which is mainly attributed to the matrix behaviour. A number of advanced micromechanics damage models have been developed by Llorca, González and co-workers (see González & Llorca (2007a), Totry *et al.* (2008a, c, b), Canal *et al.* (2009), Totry *et al.* (2009), Totry *et al.* (2010)) which predict the effects of matrix non-linearity as well as fibre-matrix debonding at the interface. In this series of papers, Llorca, González and co-workers carry out numerous studies characterising the behaviour of fibre reinforced composites when subjected to transverse tensile loading (Canal *et al.* 2009), transverse compressive loading (González & Llorca 2007a, Totry *et al.* 2008a) and transverse shear loading (Totry *et al.* 2008a, Canal *et al.* 2009). These analyses were carried out on RVEs which contained approximately 30 randomly distributed circular fibres, where it was assumed the materials under investigation had fibre volume fractions of 50%. A brief outline from these important contributions characterising composite behaviour under various loading scenarios follows.

Canal *et al.* (2009) examined the behaviour of an epoxy-modified fibre reinforced composite under transverse tensile loading. The rubber modified epoxy was modelled as an elasto-viscoplastic solid, whose behaviour was defined using a UMAT subroutine, while a cohesive zone model was implemented at the fibre-matrix interfaces to predict fibre-matrix debonding. Under transverse tensile loading, it was found that the fibre-matrix interface strength had a significant effect on transverse deformation. For a weak interface, failure initiated due to the nucleation of interface cracks which propagated along the weakest path resulting in a fracture path perpendicular to the direction of the applied transverse tensile load, as shown in Fig. 2.25 (a). Meanwhile, for a strong interface, deformation was dominated by void nucleation and growth in the rubber modified epoxy matrix (not shown). In González & Llorca (2007a), the behaviour of a carbon fibre/epoxy composite was examined under transverse compression in a similar RVE to that used by Canal *et al.* (2009). The non-linear behaviour of the epoxy matrix was implemented using a Mohr-Coulomb plasticity model, while a cohesive zone model at the fibre-matrix interface was used to predict fibre-matrix debonding. It was found that the transverse compressive properties were controlled by the interface strength and matrix compressive yield strength. The interface strength controlled the yield strength of the material while the interface fracture energy controlled the progression of damage. Here, the Mohr-Coulomb model provided an
accurate description of matrix deformation as it captured the same orientation of the fracture plane as experimental observations, as shown in Fig. 2.25 (b).

![Figure 2.25: (a) Transverse tensile deformation in a fibre reinforced rubber modified epoxy composite (load applied in the vertical direction) (from Canal et al. (2009)) and (b) transverse compressive deformation of a fibre reinforced epoxy composite with a strong fibre matrix interface (from González & Llorca (2007a)).](image)

Totry et al. (2008a) examined the behaviour of carbon fibre/epoxy composite under transverse shear loading using the same description of constituent material behaviour as in González & Llorca (2007a). Under transverse shear loading, failure was found to depend on the relative strength of the fibre-matrix interface and the yield stress of the matrix. For a strong interface, failure was found to be dominated by the propagation of a plastic shear band in the matrix which localised after the peak stress, as shown in Fig. 2.26 (a). For a weak interface, the transverse shear strength was reduced and failure was dominated by a series of interface cracks, which coalesced due to significant plastic strain in the intermediate matrix regions, as shown in Fig. 2.26 (b).

![Figure 2.26: Transverse shear deformation of a carbon fibre/epoxy composite for (a) a strong fibre-matrix interface and (b) a weak fibre matrix interface (legend indicates plastic strain), (from Totry et al. (2008a)).](image)
These advanced micromechanics damage models also allow for the prediction of complex material failure surfaces by subjecting the micromechanical models to combined loading scenarios. Totry et al. (2008a) used a combined transverse compressive and shear loading regime to determine the material failure surface of a carbon fibre/epoxy composite. This was carried out for both a weak and strong fibre-matrix interface. Again, the fibre-matrix interface strength had a significant effect on the composite failure strength as the failure locus from a weak fibre-matrix interface predicted much lower failure strengths as the case which considered a strong fibre-matrix. The difficulties associated with the multi-axial mechanical testing of this type of loading regime on a composite lamina means that virtual testing using computational micromechanics is emerging as an alternative approach for failure based predictions.

2.7 Discussion of Literature Review

2.7.1 Introduction

In this chapter, a comprehensive literature review was carried out on work relating to the micromechanical modelling of damage and failure in fibre reinforced composites. Firstly, the review focussed on defining a suitable representative volume element, whose local morphology was statistically equivalent to experimental composite microstructures. Secondly, the review highlighted the effect of the constituent material properties on local damage processes and outlined a number of current micromechanical damage models which effectively accounted for these effects. This final section discusses the main findings from the reviewed literature and their impact on work carried out in the remainder of this thesis.

2.7.2 Damage and Failure in Composite Materials

In Section 2.2.1, the complex nature of damage progression in composite laminates was highlighted. In particular, it was shown that failure in the material is a consequence of local failures occurring at the intra-ply level. Through the process of damage accumulation, microscopic damage mechanisms coalesce to cause failure at the ply level and above. It is important to note that ply failure is generally a result of multiple local damage mechanisms occurring, meaning the interaction of local damage
mechanisms during the failure process presents a number of challenges for accurate numerical predictions.

It was shown in Section 2.2.2 that current numerical strategies used to predict damage and failure in composite laminates are based on the continuum approach which only predicts the effect of ply degradation mechanisms, i.e. stiffness loss and permanent plastic strain. These models do not account for the physical damage mechanisms responsible for ply failure, or indeed the interaction of these damage mechanisms and the local stress concentrations associated with discrete micro-cracking processes. While a number of these models are highly advanced and have been shown to be reasonably accurate, given the complexity of the failure process being analysed, computational micromechanics provides the distinct advantage of predicting the onset and evolution of microscale damage and determining its effect at higher length scales. This facilitates a better understanding of local damage processes in composite plies and allows for novel insight from both a material science and an engineering viewpoint.

2.7.3 Micromechanical Modelling of Composites

Section 2.3 outlined the widely used periodic homogenisation model and the concepts of localisation and homogenisation to analyse heterogeneous materials on multiple scales. The early definition of the RVE put forward by Hill (1963) led to the development of periodic fibre unit cells, from which accurate predictions of homogenised properties could be obtained, such as those by Sun & Vaidya (1996). However, experimental studies by Pyrz (1994a) and Lewandowski et al. (1989) showed that materials which exhibited clustered reinforcements were more likely to suffer damage onset. As fibre reinforced composites generally exhibit a non-uniform material microstructure, these findings suggested that the fibre arrangement would have a distinct effect on formation and subsequent propagation of local damage mechanisms.

Using computational micromechanics, a number of authors, namely Brockenbrough et al. (1991), Böhm et al. (1993), Trias et al. (2006b), Hojo et al. (2009), compared the performance of periodic fibre unit cells with non-uniform RVE models and in all cases it was shown that periodic fibre unit cells could not represent the microscopic stress state under transverse tensile loading. In particular, Hojo et al. (2009) found that the magnitude of the interfacial stresses were significantly increased
when the inter-fibre spacing was less than 0.5µm. As a consequence, more recent definitions of the RVE, such as those by Swaminathan et al. (2006), require correlation of statistical distributions describing the fibre arrangement, allowing for a more accurate resolution of local microscopic stress and strain fields. This means that any micromechanical model which predicts damage and failure should have a fibre distribution which is statistically equivalent to the actual microstructure under consideration.

### 2.7.4 Analysis of Fibre Distribution in Composite Microstructures

Section 2.4 outlined a number of issues regarding the numerical generation of non-uniform fibre distributions for micromechanical modelling. In order to account for the non-periodic nature of composite microstructures, a number of authors have used the hard-core model to generate a random distribution of fibres in the RVE (Yang et al. 1997). However, this model cannot recreate microstructures seen in high strength composite laminates, as it reaches a saturation point at 54% fibre volume fraction. The difficulty of generating high volume fraction fibre distributions has meant that a number of studies have been carried out on high strength composites using RVEs which have assumed an incorrect fibre volume fraction. For example, Trias et al. (2006b) analysed the behaviour of a high strength carbon fibre/epoxy composite with a fibre volume fraction of 60% by assuming a hard-core fibre arrangement with a fibre volume fraction of only 50%. Numerical approaches have been developed which overcome the hard-core model’s intrinsic jamming limit, such as those proposed by Melro et al. (2008) and Wongsto & Li (2005), but these require complicated fibre stirring/shaking algorithms to be introduced in order to achieve high volume fractions. These numerical methods also assume that the microstructure of a composite material is exclusively described by a random pattern. As was shown by Pyrz (1994b), this is not always the case, as the type of pattern present depends on the manufacturing and processing conditions of the composite. The alternative is to use a microstructure reproduction approach, as used by Trias et al. (2006a). However, this approach presents difficulties in the application of periodic boundary conditions as microstructures are rarely geometrically periodic (through the boundaries).

Thus, due to the shortcomings of both numerical and experimental approaches outlined, it would be beneficial to develop a combined experimental-numerical
approach for generating statistically equivalent representations of a high strength composite laminate. It was shown by both Pyrz (1994a) and Hojo et al. (2009) that the nearest neighbour distances between fibres had a considerable effect on the microscopic stress state. This means that for accurate damage prediction, the short range interaction of fibres needs to be accurately reproduced in the micromechanical model. Thus, this thesis aims to adopt a bottom-up approach, whereby the experimentally measured nearest neighbour distribution functions will be used to define the inter-fibre distances in the micromechanical model. This should allow the short range interaction of fibres in the microstructure to be reproduced, enabling an accurate representation of the local microscopic stress state. Using techniques described in Buryachenko et al. (2003), the microstructure of composites can be characterised and statistical data, such as radial distribution functions and second order intensity functions can be found. These functions offer a quantitative measure of both short and long range interaction of fibres and, as a result, correlation of these functions between the micromechanical model and the experimental microstructure will be important for accurate predictions of local stress fields.

The size of the RVE is also an important issue to consider as there has been a large variance in the size used across the literature. For example, the significant difference in the size of RVE used by Trias et al. (2006c) and by González & Llorca (2007a) is a result of the analysis being carried out. Trias et al. (2006c) carried out a linear elastic analysis to examine the probability of matrix cracking whereas González & Llorca (2007a) required a sufficiently dense mesh to implement non-linear material behaviour coupled with a cohesive zone model at the interface to predict fibre-matrix debonding. It is therefore apparent that the size of RVE is dependant on the complexity of the problem being analysed and so, the selection of a suitable sized RVE should allow a sufficient mesh density to resolve local deformation fields adequately while maintaining relatively efficient computational run times.

2.7.5 Effect of Constituent Materials on Mechanical Behaviour

Section 2.5 outlined a number of issues regarding the constituent materials and how their adhesion to one another during the curing process affects material behaviour. The yielding behaviour of epoxy resins was shown by Asp et al. (1996b) and Fiedler et al. (2001b) to be dependant on the hydrostatic stress and as a result it was found that
pressure insensitive yield criteria, such as Von Mises, do not provide a suitable prediction of post yield behaviour. The dilatational energy density criterion proposed by Asp et al. (1996a) provides a suitable description of matrix failure under transverse tensile loading due to the largely hydrostatic stress state present in the matrix. The criterion has been used by others (Fiedler et al. 2001b, Trias et al. 2006a) to predict matrix initiated failure under transverse tensile loading, however, its application to shear dominated stress states is questionable as it does not consider the contribution of the deviatoric stress component, which is known to influence shear yielding behaviour. Meanwhile, the Mohr-Coulomb yield criterion has been shown to provide a good description of the epoxy yield behaviour for a wide range of complex combined loading scenarios. The Mohr-Coulomb model provides the added advantage that it can be calibrated with only the tensile and compressive strengths of the material.

It was also shown in Section 2.5 that the transverse strength of a composite material is dependant upon the properties of the fibre-matrix interface. Both Hinz et al. (2009) and Gamstedt & Sjögren (1999) showed that through damage accumulation, fibre-matrix debonding could subsequently lead to a number of other damage mechanisms, such as delamination or fibre fracture in neighbouring plies. Berglund and co-workers (Varna et al. 1997, Zhang et al. 1997) have shown that the use of coupling agents can increase both the strength and toughness of the fibre-matrix interface. However, this study also highlights the possible variance in the fibre-matrix interface parameters for different composite material systems.

Thermal residual stresses formed during the curing process were shown to have little effect on the stiffness of the composite but can greatly influence the failure behaviour both positively and negatively, depending on the loading condition. Thermal residual stress has been shown to have largely beneficial effects on the transverse tensile strength by numerous authors (Hojo et al. 2009, Maligno et al. 2008) due to the large compressive stresses which develop during the cool-down from cure temperature. However, for shear dominated loading, Zhao et al. (2006) showed that material strength is reduced due to increased shear stress acting at the interface. It should be noted that many of these investigations have used either a linear elastic analysis (Hojo et al. 2009) or simple periodic fibre unit cells (Zhao et al. 2006, Maligno et al. 2008) to examine the effects of thermal residual stress. Also, following the findings of Gentz et al. (2004), who observed interfacial damage occurring during the curing process, it would be
interesting to examine the potentially harmful effect the curing process can have on the material, particularly at the fibre-matrix interface.

This review has revealed that the micromechanical response is dependant upon numerous contributing factors, such as constituent properties, interfacial properties, and the presence of thermal residual stresses. This thesis aims to examine, in detail, the effects of these intra-ply properties on material behaviour using an advanced micromechanics damage model. This model will be used to predict local deformation processes, such as matrix yielding and fibre-matrix debonding, under a range of thermal/mechanical loading scenarios, which will provide novel insight into the microscopic damage that forms prior to ultimate failure. In particular, this review has shown that fibre-matrix debonding is incipient to numerous other microscopic damage mechanisms and that the properties at the fibre-matrix interface can vary considerably, depending upon processing conditions and the presence of surface treatments. Consequently, for the work carried out in this thesis, it would be prudent to examine a large range of interface strength/toughness values to fully characterise their effect on the material response.

2.7.6 Micromechanics Damage Models

In Section 2.6, a number of micromechanics damage models were reviewed, together with their findings on how microscale deformation affected macroscopic material behaviour. The non-selective stiffness degradation scheme used by both Zhao et al. (2006) and Maligno et al. (2008, 2009, 2010) to model micro-cracking assumed a reduction in the material stiffness to 1% of its original value, following the onset of damage. This represents highly brittle behaviour and essentially assumes that the fracture toughness of the material is negligible and is therefore very far removed from the more widely used cohesive zone model. Both Ghosh et al. (2000) and Kushch et al. (2010) implemented a cohesive zone model at the fibre-matrix interface to predict fibre-matrix debonding in a random fibre RVE model and assumed linear elastic behaviour of the matrix. Cid Alfaro et al. (2010) advanced this to implement a cohesive zone model between the continuum elements in the epoxy matrix, as well as a cohesive zone model at the interface to predict debonding. Importantly, these studies demonstrate the ability of the cohesive zone model to predict similar crack formations as experimental observations.
While the above models provide an adequate description of constituent material behaviour under transverse tensile loading, the micromechanical model developed by Llorca, González and co-workers has been used to examine material behaviour over a range of uniaxial and multiaxial stress states. These advanced micromechanical models used a cohesive zone model to predict the onset of fibre-matrix debonding and, importantly, predict non-linear behaviour of the epoxy matrix using the Mohr-Coulomb plasticity theory. As discussed in Section 2.5, the Mohr-Coulomb criterion accounts for the dependence of the yield stress of an epoxy on the hydrostatic pressure. Importantly, Llorca, González and co-workers show that the Mohr-Coulomb model provided an accurate description of matrix deformation under compressive loading, as it captured the same orientation of the fracture plane as experimental observations. These investigations have also established the important role the fibre-matrix interface plays in determining the overall material response. In general, they showed that the strength of the fibre-matrix interface had a distinct effect in determining the overall strength of the material.

While these models have been used to examine a number of loading scenarios in the transverse plane (González & Llorca 2007a and Totry et al. 2008a), it was shown in Section 2.3-2.5 that the micromechanical behaviour depends upon a multitude of contributing factors. These include constituent properties, interface strength, interface toughness, fibre volume fraction, local fibre distribution and the presence of thermal residual stresses. Few, if any, micromechanical investigations have considered the effects of all of these factors, in particular the effect of thermal residual stress, on microscopic damage evolution in high strength composites (~60% fibre volume fraction). By developing a novel method to generate high fibre volume fraction statistically equivalent RVEs, this thesis aims to comprehensively investigate the effect of all such factors on microscale deformation processes, under both transverse tensile and transverse shear loading. This thesis will implement a similar computational framework to that pioneered by Llorca, Gonzáles and co-workers (González & Llorca 2007a, Totry et al. 2008a) whereby, a cohesive zone model will be used to predict the onset of fibre-matrix debonding, while the non-linear behaviour in the matrix phase will be modelled using the Mohr-Coulomb plasticity theory.
Chapter 3

Generating Statistically Equivalent Fibre Distributions for High Strength Composites

3.1 Introduction

In this chapter, an algorithm is developed which is capable of generating statistically equivalent fibre distributions for a high strength carbon fibre/epoxy composite. As discussed in Chapter 2, the microstructure of a fibre reinforced composite material generally exhibits a non-uniform spatial arrangement of fibres. Numerous micromechanical investigations have shown that the local stress/strain fields depend greatly upon the local fibre arrangement (Trias et al. 2006b, Hojo et al. 2009) and therefore the use of traditional periodic fibre unit cells (Sun & Vaidya 1996), which assume a regular fibre arrangement within the microstructure, are not suitable for the prediction of damage and failure. To capture the non-uniform spatial arrangement of fibres within a composite microstructure, a sufficiently large multi-fibre Representative Volume Element (RVE) is generally used. The RVE should exhibit the same effective stress-strain behaviour as the overall material and the distribution functions reflecting the local morphology should be equivalent to the actual microstructure (Swaminathan et al. 2006).
Here, a method is proposed which uses a combined experimental-numerical approach for generating statistically equivalent fibre distributions of a high strength composite laminate. Because of the nature of high volume fraction composites, fibres are forced to arrange themselves in close proximity to one another, commonly at distances less than 0.5µm, resulting in a significant increase in the magnitude of the interfacial stresses (Hojo et al. 2009), which are a key factor in transverse failure. The approach taken here uses experimentally measured nearest neighbour distribution functions to define the distances between fibres and an experimentally measured diameter distribution function to assign fibre diameters. This allows the short range interaction of fibres in the microstructure to be reproduced, enabling an accurate representation of the local microscopic stress state. The approach is verified against a number of statistical and mechanical criteria.

This chapter is organised as follows. In Section 3.2, the microstructure of the material under investigation is experimentally characterised using digital image analysis. Section 3.3 presents the statistical distributions describing the spatial arrangement of fibres within the composite microstructure. Section 3.4 describes the newly developed algorithm which is capable of generating statistically equivalent fibre distributions for a high strength carbon fibre/epoxy composite. Section 3.5 verifies that the distributions produced by the new algorithm are indeed statistically equivalent to those of the real material. Section 3.6 verifies the mechanical behaviour of the numerically generated microstructures. Finally, Section 3.7 provides the concluding remarks on the work carried out in this chapter.

Note: The findings from Chapter 3 have been published as a peer-reviewed journal article in Composites Science and Technology under the title, *A combined experimental-numerical approach for generating statistically equivalent fibre distributions for high strength laminated composite materials* (Vaughan and McCarthy 2010).

### 3.2 Experimental Characterisation of Fibre Arrangement

The material under study is HTA/6376, a high strength carbon fibre reinforced plastic (CFRP) used extensively in the aerospace industry. The microstructure was
characterised using standard microscopy techniques along with digital image analysis, the procedures for which are described below.

3.2.1 Sample Preparation

The analysis was carried out on a 2 mm thick, 16-ply unidirectional composite laminate. A small section (i.e. 15mm × 10mm) was cut from a relatively large panel using a diamond coated circular saw blade. The sample was then mounted in a clear epoxy resin, such that the direction of grinding was perpendicular to the unidirectional fibres. The grinding process involved 600 and 1200 grit silicon carbide paper, followed by polishing stages using diamond suspensions of 6µm and 1µm. A final polishing stage was carried out using 0.05µm alumina suspension fluid.

3.2.2 Digital Image Analysis

Digital image analysis was carried out using Buehler Omnimet imaging software. In order to characterise the microstructure of the composite material, 40 images, like that shown in Fig. 3.1 (a), were captured. Each measured 320µm × 240µm and contained approximately 1,300 fibres. The software can automatically detect a colour ‘threshold’ level within each image and this allowed it to identify the fibres, as shown in Fig. 3.1 (b). From the image, the software extracted information such as fibre diameter and x,y coordinates of each fibre centre (note: only fibres which lay entirely in the view field were considered).
Figure 3.1: Sample image chosen for analysis (320 µm × 240 µm), (a) actual micrograph, (b) computed microstructure based on a colour threshold algorithm.

3.3 Statistical Characterisation of CFRP Microstructure

The data extracted from the digital image analysis was used to generate statistical functions that characterise the CFRP microstructure. Figure 3.2 shows the distribution of fibre diameters, which conformed to a lognormal distribution, as shown. The mean fibre diameter is 6.6 µm and the fibre volume fraction \( V_f \) was computed as 59.2%. As discussed in Chapter 2, many statistical descriptors exist which characterise spatial point patterns (Diggle 2003) and these can be applied to the microstructural arrangement in composite materials by considering the positions of all fibre centres as a spatial point
pattern. Three statistical descriptors are considered here which analyse both the short and long range interaction of inclusions and these are discussed below.

![Fibre diameter distribution fit to a lognormal distribution curve.](image)

**Figure 3.2:** Fibre diameter distribution fit to a lognormal distribution curve.

### 3.3.1 Nearest Neighbour Distributions

Nearest neighbour distribution functions detail the short range interaction between fibres by analysing the distance between each fibre and their $n^{th}$ closest neighbour (Diggle 2003). Shown respectively in Figs. 3.3 (a) and (b) are the 1$^{st}$ and 2$^{nd}$ nearest neighbour distributions of fibres. These distributions exhibit narrow ranges and high peaks occur at distances of 7µm and 7.2µm, respectively. From Fig. 3.2, the mean of the diameter distribution was found to be 6.6µm which implies that, for neighbouring fibres, the average inter-fibre spacing is in the region of 0.4µm-0.6µm. This minimal spacing between fibres has been shown by Hojo et al. (2009) to have a significant effect on the stresses developed at the fibre-matrix interface under transverse tensile loading, which will affect the overall failure properties of the composite. This further highlights the importance of reproducing these characteristics in a micromechanical model.
3.3.2 Radial Distribution Function

The average fibre density varies as a function of distance from a given fibre centre. The radial distribution function, \(G(r)\), shown in Fig. 3.4, exhibits a large peak at a distance of 7\(\mu\)m, which coincides with the peak seen in the 1\(^{st}\) nearest neighbour distribution function (shown in Fig. 3.3(a)). For the medium range (i.e. \(10\mu\text{m} \leq r \leq 25\mu\text{m}\)), the function exhibits some fluctuations, typical of a high volume fraction composite, due to the physical area taken up by the fibres. At the long range (i.e. \(r > 25\mu\text{m}\)), the function

![Figure 3.3: Experimentally measured nearest neighbour distances (a) 1\(^{st}\) nearest neighbour distribution function (b) 2\(^{nd}\) nearest neighbour distribution function.](image)
approaches unity as the value of \( r \) becomes large enough to be representative of the overall region, indicating that the microstructure is statistically homogeneous.

![Figure 3.4: Radial distribution function for the composite.](image)

### 3.3.3 Second-Order Intensity Function

The second-order intensity function, also described in Section 2.4.1, is widely used to distinguish between different types of point patterns (Pyrz 1994b). Shown in Fig. 3.5 are the second-order intensity functions for the CFRP composite and a distribution which exhibits Complete Spatial Randomness (CSR). It can be seen that the experimental curve is initially below the CSR curve and shows evidence of a slight stair-shape, which is indicative of a certain amount of regularity in the fibre arrangement at shorter distances (i.e. \( r \leq 15 \, \mu m \)). However, at larger distances (i.e. \( r > 15 \, \mu m \)) the curve is above and diverging away from the CSR pattern, which is a result of long range clustering. It can be thus concluded that the distribution of fibres in CFRP microstructure does not conform to a CSR pattern. This then rules out the approaches outlined earlier which generated a random distribution of fibres and highlights the need to develop an approach that can recreate the spatial pattern of the actual experimental microstructure.
3.4 Nearest Neighbour Algorithm (NNA)

Following this finding, an algorithm was developed in MATLAB and its purpose was to generate a high volume fraction fibre distribution which is statistically equivalent to the actual CFRP microstructure.

3.4.1 Algorithm Description

The importance of the short range interaction of fibres has already been highlighted and to accurately reproduce this, the algorithm uses a bottom-up approach by populating a region using an ‘adjusted’ measure of the 1st and 2nd nearest neighbour distribution functions, shown in Figs. 3.3 (a) and (b), respectively, to define the distances between neighbouring fibres. This adjusted measure is needed because of the fact that a nearest neighbour distance may be shared by 2 fibres, such as Fibre A and Fibre B, shown in Fig. 3.6. When measuring the nearest neighbour distribution function, this distance is accounted for twice (i.e. Fibre A’s nearest neighbour is Fibre B, and vice-versa). In order for the newly developed algorithm to reproduce equivalent distribution functions, the nearest neighbour distances common to two fibres may only be counted once. For example, for Fibre B, instead of using the distance to Fibre A (which has already been counted in the distribution as Fibre B is Fibre A’s nearest neighbour), the distance between it and Fibre C is now counted in the adjusted nearest neighbour distribution. This follows for all fibres under consideration. The resulting adjusted measures of the 1st and 2nd nearest neighbour distributions, shown in Figs. 3.7.
(a) and (b), respectively, exhibit very similar properties to the original nearest neighbour distributions (shown in Figs. 3.3 (a) and (b)). The adjusted first and second nearest neighbour distribution functions could both be fit to logistic distribution curves, as shown in Figs. 3.7 (a) and (b).

Figure 3.6: 'Adjusted' measure of the nearest neighbour distribution function.

![Diagram](image)

Figure 3.7: Logistic distributions fit to the 'adjusted' measures of the (a) 1st nearest neighbour distribution and (b) 2nd nearest neighbour distribution.
The algorithm then uses these logistic distribution parameters to define the inter-fibre distances for the first and second nearest neighbours of a given fibre. Fibre diameters are chosen directly from the experimentally measured fibre diameter distribution curve, shown in Fig. 3.2. The algorithm, known as the Nearest Neighbour Algorithm (NNA), follows the procedure outlined below, while the actual MATLAB code (.m file) is contained in Appendix B.

1. A random point is created having coordinates \((x_1, y_1)\), lying in a sample square area, \(A\); the size of \(A\) being defined by the user. The diameter, \(d_1\), of the surrounding fibre is drawn from a lognormal distribution fitting the experimentally measured diameter distribution, shown in Fig. 3.2.

2. A second point is created \((x_2, y_2)\), which is the centre of the first nearest neighbour of the previous fibre. The distance from \((x_1, y_1)\) to \((x_2, y_2)\) is assigned from the adjusted first nearest neighbour distribution function, shown in Fig. 3.7 (a). The new point is oriented at a random angle \(\theta_1\), where \(-\pi \geq \theta_1 \geq \pi\) (see Fig. 3.8). The fibre diameter is assigned from the same lognormal distribution as before.

3. A third point is created \((x_3, y_3)\), which is the centre of the second nearest neighbour of the first fibre. The distance from \((x_1, y_1)\) to \((x_3, y_3)\) is assigned from the adjusted second nearest neighbour distribution function, shown in Fig. 3.7 (b). As before, the new point is oriented at a random angle \(\theta_2\), where \(-\pi \geq \theta_2 \geq \pi\) (see Fig. 3.9) and the fibre diameter is assigned from the lognormal distribution, as before.
4. The NNA then moves on to the second fibre and assigns its first and second nearest neighbours, for which the nearest neighbour distances are drawn from their respective distributions and fibre diameters are assigned as before (See Fig. 3.10).

5. The NNA then moves on to the third fibre and the same procedure is carried out. This process is repeated for each fibre thereafter until the sample area, $A$, is filled.

6. The NNA performs numerous checks at each iteration to ensure that none of the fibres overlap with one another and the fibres lie within the sample area chosen. If overlaps occur or a fibre is placed outside the sample area, orientation angles or inter-fibre distances are reassigned until a suitable configuration is found.

7. If no suitable configuration can be found (i.e. near a boundary or in a region saturated with fibres), the NNA will move on to the next fibre and continue as before.

8. For any fibre crossing a boundary, a corresponding fibre is placed on the opposing boundary to maintain geometric periodicity. A fibre already situated in this area will be removed if an overlap occurs with the newly mapped fibre. However, a new fibre is subsequently reassigned a position near the mapped
fibre should it be available in order to try and maintain the correct fibre volume fraction locally.

It should be noted that a minimum inhibition distance of 0.1µm between neighbouring fibres was specified to allow for adequate discretisation in the inter-fibre region for subsequent finite element modelling. Figure 3.11 shows a view of a sample microstructure which is in the process of being generated by the NNA. In Figs. 3.11 (a)-(f), a snapshot has been taken at different fibre volume fractions throughout the generation process. This microstructure measures 165µm ×165µm.

![Figure 3.11](image)

Figure 3.11: NNA in the process of generating a sample microstructure measuring 165µm ×165µm with snapshots taken at (a) 10% \( V_f \) (b) 20% \( V_f \) (c) 30% \( V_f \) (d) 40% \( V_f \) (e) 50% \( V_f \) and (f) 60% \( V_f \).

### 3.5 Statistical Characterisation of Nearest Neighbour Algorithm

In order to analyse the numerically generated microstructures, an RVE size large enough to be representative of the bulk material must be used. The size of an RVE can be represented by the variable \( \delta \), which relates length of the side of the RVE \( L \), to the fibre radius \( r_f \), using the following simple relationship,
Trias et al. (2006c) determined that for a typical carbon fibre reinforced plastic, having a fibre volume fraction of 50%, the minimum required size of an RVE is $\delta \geq 50$. The mechanical and statistical criteria considered for the analysis were the effective properties, the Hill condition, the mean and variance of stress and strain fields, probability density functions of the stress and strain components in the matrix and fibre distance distributions.

Following this study, a value of $\delta=50$ was used to generate 20 microstructures each measuring 165µm x 165µm and one of these is shown in Fig. 3.12 (a). A microstructure exhibiting a periodic hexagonal array of fibres (with the same fibre volume fraction) is also shown in Fig. 3.12 (b). This type of arrangement would have been the focus of many previous micromechanical investigations of composite materials (Maligno et al. 2008). The microstructure generated by the NNA is seen to reproduce short range regularity, matrix rich regions and ‘lines’ of fibres much the same as in the original micrograph, shown in Fig. 3.13. Four regions (A, B, C and D) have been identified in both images to highlight these similarities. The statistical descriptors (discussed in Section 3.3) characterising these models have been derived and the mean values for these arrangements are compared to the experimentally measured statistical functions. Error bars have been included for each of the functions indicating the maximum and minimum values generated from the models for each data point and are discussed next.
3.5.1 Nearest Neighbour Distributions

Shown in Fig. 3.14 (a) and (b) are the probability density functions for the 1\textsuperscript{st} and 2\textsuperscript{nd} nearest neighbour distances, respectively. As these formed some of the input parameters for the NNA, a very good correlation is found between the experimentally measured distribution and the distributions generated by the NNA, thus showing that the short range interaction of fibres is being accurately reproduced. This has important implications when modelling damage and failure in composites as the highest stresses tend to occur in regions where fibres are in closest proximity.
The radial distribution functions for both the numerically generated microstructures and the experimental microstructure are shown in Fig. 3.15. Again, excellent correlation is achieved, thus confirming that the NNA is reproducing the same short and long range inter-fibre distances. The graph shows an initial high peak caused by the physical area of the inclusions, followed by a number of oscillations until, finally, the value of the plot approaches a value of unity, indicating the numerically generated microstructures are statistically homogenous.

3.5.2 Radial Distribution Function

The radial distribution functions for both the numerically generated microstructures and the experimental microstructure are shown in Fig. 3.15. Again, excellent correlation is achieved, thus confirming that the NNA is reproducing the same short and long range inter-fibre distances. The graph shows an initial high peak caused by the physical area of the inclusions, followed by a number of oscillations until, finally, the value of the plot approaches a value of unity, indicating the numerically generated microstructures are statistically homogenous.
3.5.3 Second-Order Intensity Function

Figure 3.16 shows the second-order intensity function (Ripley’s $K$-function) for the experimental microstructure and the numerically generated microstructures. Also shown is the second-order intensity function for a model which exhibits complete spatial randomness. Excellent agreement is seen in the type of pattern being generated by the NNA and the experimental microstructure. The NNA is able to replicate the regularity between fibres in the real microstructure at short range distances, indicated by the slight stair shape seen in the plot at smaller values of $r$. The CSR pattern does not replicate this initial stepwise increase. At larger distances the curve diverges away from the CSR pattern, reproducing the long range clustering from the experimental sample. Thus, the same spatial pattern is being produced by the NNA, for which the statistical distributions defining it are almost identical.
As the nearest neighbour distribution functions were used to define inter-fibre distances, it would be expected that the short range interaction of fibres would be reproduced (seen in Figs. 3.14 (a) and (b)) However, correlation of the long range inter-fibre distances and overall pattern being produced may not have necessarily followed. The correlation of both short and long range inter-fibre distances validates the bottom-up approach that the NNA uses to generate distributions for high volume fraction composites. Thus, the distributions being generated are statistically equivalent to the real microstructure of the CFRP composite.

### 3.5.4 Fibre Volume Fraction

Unlike other similar algorithms (Melro et al. 2008), the fibre volume fraction of the numerically generated microstructures is not predefined. It is controlled by the experimental functions used as the input parameters, i.e. the adjusted nearest neighbour distributions and the diameter distribution of the fibres. In order to test the effectiveness of the NNA, the fibre volume fraction has been examined over a range of RVE sizes, as shown in Fig. 3.17. Twenty microstructures were generated at each value of \( \delta \) and it can be seen that there is a large variance between the fibre volume fractions produced for the smallest models (i.e. \( \delta = 10 \)). This is due to the relative size of the fibres compared to the overall RVE window size and the conditions the NNA uses when placing fibres near a boundary. For smaller models, the influence of the boundary is relatively large.
compared to the overall area of the RVE. The larger models (i.e. $\delta \geq 20$), are seen to converge close to the experimental fibre volume fraction of 59.2% showing very little variance in the fibre volume fractions being produced.

![Image](image.png)

Figure 3.17: Fibre volume fraction size study.

### 3.5.5 Model Generation Time

The simulations were carried out on a desktop workstation which had a 2.13GHz Intel® Core™ 2 Duo CPU and 3.5GB of RAM. The mean running time to generate the numerical microstructures (where $\delta=50$) using the NNA was 4.01mins. Thus, a relatively quick and efficient method has been developed to generate numerical microstructures having a high fibre volume fraction. In contrast, Trias (2005) developed an algorithm based on the random close packing of spheres and a typical run time to generate similar fibre volume fractions was in excess of 120mins.

### 3.6 Prediction of Effective Properties

As outlined in Chapter 2, micromechanics based simulations of heterogeneous materials allow for the prediction of the macroscopic response through the application of appropriate boundary conditions. Micromechanics can also predict microscopic state variables (i.e. local stress and strain fields) enabling a comprehensive understanding of the contribution of each constituent phase and how their interaction affects the
macroscopic behaviour. For the present analysis, the periodic homogenisation approach is used to determine a set of effective properties from a number of RVEs generated by the NNA, in order to verify their mechanical behaviour.

### 3.6.1 Periodic Boundary Conditions

Periodic boundary conditions, similar to those used by Van der Sluis et al. (2000), have been used to ensure a macroscopically uniform stress/strain field is imposed on the RVE, allowing effective macroscopic behaviour to be determined for a given loading condition. The periodic boundary conditions require opposing boundaries of the RVE be compatible, meaning that boundary pairs undergo identical deformations. For this reason, the microstructures generated by the NNA are geometrically periodic such that, any fibre which penetrates the boundary of the RVE has a corresponding fibre situated on the opposite boundary, as shown in Fig. 3.12 (a). For the finite element simulations, the periodicity assumption also requires that the nodesets on each boundary pair be identical. The ‘advancing front’ meshing algorithm was used for this purpose and a section of the resulting opposing nodesets is shown in Fig. 3.18, where nodes in the West Nodeset are paired to nodes opposite them in the East Nodeset. The periodic boundary conditions are implemented using a series of constraint equations, through the *EQUATION keyword in ABAQUS, along with displacements applied to control nodes enabling the relevant modes of deformation in an RVE to be simulated. In two-dimensions, the periodic boundary conditions used to determine the effective response of a geometrically periodic RVE can be expressed in terms of the nodal displacement vector, \( \mathbf{u} \), such that,

\[
\begin{align*}
\mathbf{u}_{\text{north}} - \mathbf{u}_{n_1} &= \mathbf{u}_{\text{south}} - \mathbf{u}_{n_1} \\
\mathbf{u}_{\text{west}} - \mathbf{u}_{n_1} &= \mathbf{u}_{\text{east}} - \mathbf{u}_{n_2}
\end{align*}
\]

where the subscripts \text{North}, \text{South}, \text{East} and \text{West} correspond to nodes situated on each edge of the RVE and subscripts \( n_1, n_2 \) and \( n_4 \) correspond to the control nodes which are located at each corner of the RVE, as shown in Fig. 3.18. In the Finite Element (FE) models, rigid body motions were eliminated by constraining the displacement of \( n_1 \) in all directions, thus reducing the above constraint equations to the following,
In order to simulate the relevant modes of deformation, displacements were applied to the control nodes. This was carried out for different loading configurations which are described as follows.

**Transverse Tension** ($E_{22}/E_{33}$)

The transverse moduli were determined using a two-dimensional generalised plane strain model using three-noded generalised plane strain elements (CPEG3). A transverse tensile stress state was imposed in the 2- and 3-direction by applying displacements to the control nodes $n_2$ and $n_4$, as shown in Fig. 3.19 (a) and (b), respectively.

\[
\mathbf{u}_{\text{north}} - \mathbf{u}_{n_1} = \mathbf{u}_{\text{south}} \quad (3.4)
\]

\[
\mathbf{u}_{\text{east}} - \mathbf{u}_{n_3} = \mathbf{u}_{\text{west}} \quad (3.5)
\]
Transverse Shear (\(G_{23}\))

The transverse shear modulus was determined using a two-dimensional generalised plane strain model using three-noded generalised plane strain elements (CPEG3). A transverse shear stress state was imposed by applying a displacement to the nodes \(n_2\) and \(n_4\), as shown in Fig. 3.20, in order to evaluate transverse shear modulus \(G_{23}\).

Figure 3.20: Periodic boundary conditions and resulting deformation for transverse shear.
Microstructure Generation

Longitudinal Tension ($E_{11}$)

A two-dimensional generalised plane strain model was used to determine the longitudinal modulus $E_{11}$ from the numerically generated microstructures, using three-noded generalised plane strain elements (CPEG3). The model applies an out of plane force (i.e. in the 1-direction) to the face of the RVE via the reference point (RP), as shown in Fig. 3.21, simulating a tensile stress state in the RVE.

![Figure 3.21: Periodic boundary conditions for longitudinal tension.](image)

In-Plane Shear ($G_{12}$)

To determine the in-plane shear modulus, a 3D RVE is needed. Just as the 2D case requires the opposing edges of the RVE to undergo identical deformations, the 3D case requires the opposing faces of the RVE to also undergo identical deformations. This implies that the discretisation of the opposing faces should be identical in order to apply the periodic boundary conditions. A bottom-up meshing algorithm was used to discretise the RVE, which had a nominal thickness (in this case 2 elements thick), with 6-noded wedge elements (C3D6). In three dimensions the periodic boundary conditions may be expressed in terms of the nodal displacement vector, $\mathbf{u}$, as follows,

$$u_{\text{front}} = u_{\text{back}} - u_{n_1}$$ (3.6)

$$u_{\text{top}} = u_{\text{bottom}} - u_{n_4}$$ (3.7)

$$u_{\text{right}} = u_{\text{left}}$$ (3.8)
where the subscripts \textit{Front}, \textit{Back}, \textit{Top}, \textit{Bottom}, \textit{Left} and \textit{Right} correspond to nodes situated on each of the faces of the RVE and subscripts $n_1$, $n_2$ and $n_4$ correspond to the control nodes which are located at the corners of the RVE, as shown in Fig. 3.22. This resulted in in-plane shear deformation of the RVE, which is shown in Fig. 3.23.

![Figure 3.22: Periodic boundary conditions applied to an RVE to determine the in-plane shear modulus.](image)

![Figure 3.23: Deformation of an RVE under in-plane shear loading.](image)

\subsection{3.6.2 Homogenisation Procedure}

\textit{Volume Averaged Homogenisation}

The homogenisation procedure relates the microscopic state variables, in this case the local stress and strain fields, to the macroscopic averaged quantities. In order to
evaluate the average stresses ($\bar{\sigma}_{ij}$) and strains ($\bar{\varepsilon}_{ij}$) over the RVE, the following equations from Keane (2009) were used,

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{k=1}^{n} (\sigma_{ij} V_k)$$  \hspace{1cm} (3.9)

$$\bar{\varepsilon}_{ij} = \frac{1}{V} \sum_{k=1}^{n} (\varepsilon_{ij} V_k)$$  \hspace{1cm} (3.10)

where $V$ is the total volume of the RVE, $k$ is the element number, $V_k$ is the volume of element $k$ in the finite element mesh, $n$ is the total number of elements and $\sigma_{ij}$ and $\varepsilon_{ij}$ are the $ij$ stresses and strains, respectively, in the element $k$. The effective properties can determined from the relevant stress-strain ratio for a given loading condition, i.e.,

$$E_{ij} = \frac{\sigma_{ij}}{\varepsilon_{ij}}$$  \hspace{1cm} (3.11)

**Surface Based Homogenisation**

A surface based homogenisation scheme may also be used to determine the average stresses ($\bar{\sigma}_{ij}$) and strains ($\bar{\varepsilon}_{ij}$) in the RVE. This involves computing the average stresses from surface tractions acting on the edges of the RVE. For example, for transverse tensile loading, shown in Fig. 3.24 (a), the transverse normal stress ($\sigma_{22}$) may be determined using the following relation,

$$\sigma_{22} = \frac{f_{n_2}}{L}$$  \hspace{1cm} (3.12)

where $f_{n_2}$ is the normal force acting at the control node, $n_2$, which results from the applied normal displacement ($\delta_n$) in the 2-direction, as shown in Fig. 3.24 (a), and $L$ is the length of the RVE. Meanwhile, the average strain may be determined by,

$$\varepsilon_{22} = \frac{\delta_n}{L}$$  \hspace{1cm} (3.13)

where $\delta_n$ is the applied normal displacement at the control node, $n_2$, and $L$ is the length of the RVE.
properties of the composite material, it is assumed that both the constituent phases of the 
reinforced with anisotropic carbon fibres (Toho Tenax HTA). In evaluating the effective 
properties may be determined by the relation shown in Eq. 3.11, as before.

Next, the average shear strain may be determined by

$$\bar{\gamma}_{23} = \frac{\delta_s}{L}$$

where $\delta_s$ is the total applied shear displacement and $L$ is the length of the RVE. The 
effective properties may be determined by the relation shown in Eq. 3.11, as before.

Constituent Material Properties

The material under study is HTA/6376, a high strength carbon fibre/epoxy 
composite. The material consists of an isotropic epoxy matrix (Hexcel 6376) which is 
reinforced with anisotropic carbon fibres (Toho Tenax HTA). In evaluating the effective 
properties of the composite material, it is assumed that both the constituent phases of the 
composite material behave linear elastically. The properties of the HTA fibres used for

Figure 3.24: Surface based homogenisation for an applied (a) normal displacement and (b) shear 

Similarly, for a transverse shear displacement applied at the control node, $n_2$, 
shown in Fig. 3.24 (b), the transverse shear stress may be determined using the 
following relation,

$$\bar{\tau}_{23} = \frac{f_{12}}{L}$$

where $f_{12}$ is the tangential force acting at the control node, $n_2$, which results from the 
applied shear displacement in the 3-direction, as shown in Fig. 3.24 (b), and $L$ is the 
length of the RVE. Meanwhile, the average shear strain may be determined by,

$$\bar{\gamma}_{23} = \frac{\delta_s}{L}$$

where $\delta_s$ is the total applied shear displacement and $L$ is the length of the RVE. The 
effective properties may be determined by the relation shown in Eq. 3.11, as before.

Constituent Material Properties

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composite. The material consists of an isotropic epoxy matrix (Hexcel 6376) which is 
reinforced with anisotropic carbon fibres (Toho Tenax HTA). In evaluating the effective 
properties of the composite material, it is assumed that both the constituent phases of the 
composite material behave linear elastically. The properties of the HTA fibres used for
the analysis are taken from Fiedler et al. (2005a), while the properties of the 6376 matrix are taken from Keane (2009) and both are presented below in Table 3.1.

Table 3.1: Constituent Material Properties

<table>
<thead>
<tr>
<th>Elastic Properties</th>
<th>Fibre (HTA)</th>
<th>Matrix (6376)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{11}$ (GPa)</td>
<td>238</td>
<td>3.63</td>
</tr>
<tr>
<td>$E_{22}$ (GPa)</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>$E_{33}$ (GPa)</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>$\nu_{12}$</td>
<td>0.23</td>
<td>0.34</td>
</tr>
<tr>
<td>$\nu_{23}$</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>$\nu_{31}$</td>
<td>0.03</td>
<td></td>
</tr>
<tr>
<td>$G_{12}$ (GPa)</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>$G_{23}$ (GPa)</td>
<td>7.2</td>
<td></td>
</tr>
<tr>
<td>$G_{31}$ (GPa)</td>
<td>24</td>
<td></td>
</tr>
</tbody>
</table>

3.6.3 Resulting Effective Properties

Effective properties were calculated for numerically generated microstructures of increasing size using the volume averaged homogenisation procedure. Twenty microstructures were generated using the NNA at each value of $\delta$. Figures 3.25 (a) and (b) show the mean values of the homogenised effective properties. Error bars have been included indicating the maximum and minimum values calculated at each value of $\delta$. The results show similar trends to the fibre volume fraction study carried out (see Fig. 3.17), with a large variance evident at low values of $\delta$ as a result of the wide range of fibre volume fractions, caused by boundary effects. It was determined that the effective properties converged to a constant value when $\delta=20$, where it was found that the maximum and minimum values of all 20 generated microstructures fell within 10% of the mean values. The mean homogenised effective properties of the largest models (i.e. $\delta=50$) compare well with experimentally measured elastic properties, which were taken from O'Higgins et al. (2008), as shown in Figs. 3.25 (a) and (b). At high values of $\delta$, very little variance in effective properties is seen for all generated models, with the maximum and minimum values falling within 3% of the mean values. As a comparison, effective properties have also been determined for periodic hexagonal fibre arrays (with same $V_f$) at each value of $\delta$ and these are also shown in Fig. 3.25. As can be seen these hexagonal models predict the same effective properties for all values of $\delta$, as would be expected, to which the properties predicted by the NNA converge.
However, under transverse tensile loading, the peak stresses in the NNA models were found, in some cases, to be 92% higher than those in the periodic models, suggesting that accurate predictions of both damage initiation and overall failure of the material is highly dependant on the type of fibre distribution used in a micromechanical model. Finally, Fig. 3.25 (b) also shows that the numerically generated microstructures are transversely isotropic due to fact that $E_{22}$ and $E_{33}$ converge to the same value for the largest models.

Figure 3.25: Effective properties of the numerically generated microstructures in (a) the longitudinal direction and (b) the transverse and in-plane directions (Experimental values (denoted by ‘Exp’) are taken from O’Higgins et al. (2008)).
3.7 Concluding Remarks

A novel method has been developed in order to generate accurate representations of a composite material microstructure with a high volume fraction. The microstructure of a CFRP composite was experimentally characterised in terms of fibre volume fraction, fibre diameter and also statistical distributions describing the fibre arrangement. It was found from the experimental analysis that CFRP microstructure had a fibre distribution which was not characterised by a CSR pattern. This highlighted the need for an experimental approach to be used to generate accurate fibre distributions. Using the experimentally measured data, an algorithm was developed which can generate fibre distributions with high volume fractions and the same geometric features as the experimental samples, as determined using statistical analysis. The NNA uses an adjusted measure of the experimentally measured 1st and 2nd nearest neighbour distribution functions to define inter-fibre distances. The key factor to avoid jamming of the microstructure (as seen in Buryachenko et al. (2003) and Melro et al. (2008)) was to assign both the 1st and 2nd nearest neighbours at each step in the process. Assigning only the first nearest neighbour was found not to produce the desired fibre distribution as it was also subject to a jamming limit at ~55%. Fibre diameters are assigned using the experimentally measured diameter distribution. Upon statistical analysis, the NNA was found to produce distributions which were statistically equivalent to the real microstructure, accurately reproducing both the short and long range interaction of fibres.

Using Finite Element Analysis, effective properties of the generated microstructures were calculated through an homogenisation procedure. The homogenised properties of the composite were found to show good agreement with the experimentally measured properties of O'Higgins et al. (2008). A parametric study, in which the size of the generated microstructure was varied, was carried out and it was found that the elastic moduli converged for a microstructure window which had a side of length of approximately 20 times the fibre radius, which for this material is approximately half a ply thickness (i.e. 65µm). Based on the results of this study, it has been found that the periodic hexagonal array can accurately predict the effective elastic properties of the composite. However, it has been found that peak stresses in the NNA models were 92% higher than those in the periodic models. This is in agreement with
the findings of Trias et al. (2006b) and Hojo et al. (2009), who suggested that periodic fibre models could not accurately predict the onset of failure in the material.

The algorithm developed is simple, robust, highly efficient and reproduces actual fibre distributions for high strength laminated composite materials. The distribution of fibres in a composite depends heavily on the manufacturing and processing conditions, and for this reason this newly developed method provides a useful alternative to purely numerical based models that rely on the theory of random close packing and also direct microstructure reproduction. It does not require further heuristic steps, such as those seen fibre stirring\shaking algorithms, in order to achieve high volume fraction microstructures. This method can easily be applied to other types of composite materials by characterising relevant experimental distributions.
Chapter 4

Micromechanical Modelling of the Transverse Damage Behaviour in Fibre Reinforced Composites

4.1 Introduction

In this chapter, a micromechanics damage model is used to examine the transverse damage behaviour of the carbon fibre/epoxy composite material (HTA/6376) under investigation. In laminate configurations, the importance of transverse plies is significant as they provide essential stiffness and strength to components undergoing multi-axial loading, helping to maintain structural integrity. The failure behaviour of these transverse plies has a major influence on the overall failure of composite laminates. Transverse fracture often occurs early in the loading history and as a result is one of the limiting design criteria in composite structures (Hojo et al. 2009). Experimental studies have shown that the dominant damage mechanism involved in transverse ply cracking is debonding occurring at the fibre matrix interface (Gamstedt & Sjögren 1999, Hobbiebrunken et al. 2006). The process is shown in Fig. 4.1 where, the initial failure of a carbon fibre/epoxy system was examined by Hobbiebrunken et al. (2006) using in-situ SEM experiments. Through the process of damage accumulation, fibre-matrix debonding can induce further damage in laminates such as inter-ply delamination or fibre fracture in neighbouring plies (Gamstedt & Sjögren 1999).
From the literature review carried out in Chapter 2, it was shown that the transverse fracture behaviour of composite materials is dependant upon numerous contributing factors, such as constituent properties, interfacial properties, local fibre distribution and the presence of thermal residual stresses. Due to the complex nature of damage progression, many micromechanical studies to date have focused on transverse fracture behaviour from the viewpoint of damage initiation (Asp et al. 1996b, Hojo et al. 2009). Meanwhile, a number of studies have made the assumption of a periodic fibre arrangement in the microstructure (Fiedler et al. 2001b, Hobbiebrunken et al. 2006, Maligno et al. 2010), which is not likely to be representative of actual material behaviour (Trias et al. 2006b, Hobbiebrunken et al. 2008, Hojo et al. 2009). Recently however, a number of advanced micromechanics damage models have been developed, such as those by Llorca, González and co-workers (González & Llorca 2007a, Totry et al. 2008a), which enable the prediction of microscopic damage progression and ultimate failure of a heterogeneous material. These have been achieved primarily through the use of cohesive zone models at the fibre-matrix interface, coupled with non-linear material models to describe the behaviour of the constituent phases.

Hence, the aim of this chapter is to collectively investigate the effects of thermal residual stress and fibre-matrix debonding on the transverse fracture behaviour of a fibre reinforced composite. The computational framework used to model deformation in the carbon fibre/epoxy composite is similar to that pioneered by Llorca, González and co-workers (González & Llorca 2007a, Totry et al. 2008a) where, a cohesive zone model is used to predict the onset of fibre-matrix debonding, while the non-linear behaviour in the matrix phase is modelled using the Mohr-Coulomb plasticity theory. The recently
developed Nearest Neighbour Algorithm (NNA) (Vaughan & McCarthy 2010), that can accurately reproduce a statistically equivalent fibre distribution for high volume fraction composites, is used to generate the finite element models for the analysis.

This chapter is organised as follows. In Section 4.2, the details regarding the micromechanical modelling procedure are outlined. In Section 4.3, the effect of thermal residual stress on the transverse fracture process is thoroughly examined and the effect of damage accumulation due to cyclic loading is assessed. Section 4.4 summarises the main findings and provides some concluding remarks on the studies carried out in this chapter.

Note: The findings from Chapter 4 have been published as a peer-reviewed journal article in Composites Science and Technology under the title *Micromechanical Modelling of the Transverse Damage Behaviour in Fibre Reinforced Composites* (Vaughan and McCarthy 2011a).

### 4.2 Finite Element Modelling

The material under study is HTA/6376, a high strength carbon fibre/epoxy composite manufactured by Hexcel and used extensively in the aerospace industry. In this chapter, three studies have been carried out to examine the transverse fracture behaviour of the composite material.

1) A linear elastic analysis is carried out to examine the microscopic stress state following the thermal cool-down from cure temperature. In particular, the Interfacial Normal Stress (INS) and Interfacial Shear Stress (ISS), which develop as a result of this thermal loading phase, are analysed.

2) The transverse fracture behaviour of the composite as a result of fibre-matrix debonding is examined. A number of loading cases are considered which examine the effect of thermal residual stress on the transverse fracture behaviour of the material. Parameter studies are carried out examining the influence of interfacial strength and interfacial toughness on the material behaviour.
3) The effect of cyclic loading on the transverse fracture behaviour is considered. The material is subject to a tensile/compressive loading regime and the effect of microscopic damage accumulation on the macroscopic response is analysed.

4.2.1 Generation of Micromechanical Models

As outlined in Chapter 3, the fibre distribution for the HTA/6376 material has been characterised and the Nearest Neighbour Algorithm (NNA) (Vaughan & McCarthy 2010) has been developed which enables statistically equivalent fibre distributions to be generated. A typical fibre distribution generated by the NNA is shown in Fig. 4.2 (a). The NNA uses experimentally measured nearest neighbour distribution functions to define the inter-fibre distances and an experimentally measured diameter distribution function to assign fibre diameters in the Representative Volume Element (RVE). This allows the short range interaction of fibres in the microstructure to be reproduced, enabling an accurate representation of the local microscopic stress state. From Chapter 3, the minimum size of RVE generated by the NNA which was found to be free from boundary effects was $\delta=20$.

Five separate RVEs, each statistically similar but topologically different to that shown in Fig. 4.2 (a) were generated and each measured $\delta=20$ and contained approximately 80 fibres. Previous studies suggest that this RVE size is more than sufficient in order to produce the overall macroscopic response of a composite (González & Llorca 2007a). Python scripts were used to generate two-dimensional finite element models of the RVEs in the ABAQUS finite element code. For the present analysis, the fibre and matrix regions were discretised using a quad-dominated mesh which consisted of predominantly 4-noded (CPEG4) and a relatively small number of 3-noded (CPEG3) full integration generalised plane strain elements, assuming a small strain formulation. A layer of cohesive elements (COH2D4) was introduced between the fibre and the matrix to predict the onset of fibre-matrix debonding. To ensure accurate prediction of deformation in the matrix, sufficiently dense meshes consisting of approximately 85,000 elements were used. A mesh sensitivity analysis was carried out to confirm the suitability of this level of mesh refinement, the details of which are contained in Appendix A. It should be noted that in order to prevent mesh-locking in the case of fully integrated first-order isoparametric elements, such as those used here (i.e. CPEG4 and CPEG3), ABAQUS replaces the actual volume changes at the Gauss
points with the average volume change over the entire element. Nagtegaal et al. (1974) have shown that this technique provides accurate solutions in incompressible or nearly incompressible cases.

The periodic boundary conditions, described in Chapter 3, were applied to the micromechanical models to ensure a macroscopically uniform stress/displacement field existed across the boundaries of each RVE. Two load cases are considered here, the first being a mechanical transverse tensile load imposed on the RVE by applying a horizontal normal displacement ($\delta_n$) boundary condition to the active control node, $n_2$, as shown in Fig. 4.2 (a). This is referred to throughout as the Mechanical Loading (ML) case. The

Figure 4.2: Periodic boundary conditions applied to an RVE simulating the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case.

The periodic boundary conditions, described in Chapter 3, were applied to the micromechanical models to ensure a macroscopically uniform stress/displacement field existed across the boundaries of each RVE. Two load cases are considered here, the first being a mechanical transverse tensile load imposed on the RVE by applying a horizontal normal displacement ($\delta_n$) boundary condition to the active control node, $n_2$, as shown in Fig. 4.2 (a). This is referred to throughout as the Mechanical Loading (ML) case. The
second load case considers the effects of thermal residual stresses in the micromechanical models. These are formed during cooling of the material from cure temperature (448 K) to room temperature (298K). A thermal load is invoked where a temperature change, $\Delta T = -150$ K, is applied globally to each node in the model, as shown in Fig. 4.2 (b) and this is subsequently followed by a mechanical transverse tensile load, identical to that shown in Fig. 4.2 (a). This is referred to throughout as the Thermo-Mechanical Loading (TML) case. It should be noted that the thermal loading phase allows free contraction of the control nodes and the only mechanical boundary conditions applied are to prevent rigid body motion. This means that the control node, $n_1$, is constrained in the 2- and 3-directions, while the control node, $n_2$, is only constrained in the 3-direction. While the mechanical properties of epoxies have been shown to vary with temperature, the cure temperature of the 6376 epoxy matrix under investigation is much less than the glass transition temperature ($T_G$) (Fiedler et al. 2005b). As a result, the temperature dependence of the constituent material properties is not considered herein. This assumption follows similar micromechanical investigations carried out by Hojo et al. (2009), Hinz et al. (2007) and González & Llorca (2007) who have all examined thermal residual stress in fibre reinforced composites assuming constant constituent properties regardless of temperature. For this two-dimensional case, the periodic boundary conditions applied to the RVE represent the behaviour of a unidirectional (UD) laminate. This means that inter-ply thermal residual stresses, which would be generated during the manufacturing process due to plies having different orientations, are not considered (e.g. in cross-ply laminate configurations).

4.2.2 Material Behaviour

HTA Fibres

The HTA fibres are assumed here to be linear elastic. It is further assumed that as loading occurs in the transverse plane, fibre fracture does not occur and thus no damage model has been implemented for the fibres. The fibres’ thermal and mechanical properties used in the analysis were taken from (Fiedler et al. 2005a) and are listed in Table 4.1.
Table 4.1: Constituent Thermo-Mechanical Properties

<table>
<thead>
<tr>
<th>Elastic Properties</th>
<th>Fibre (HTA)</th>
<th>Matrix (6376)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{11}$ (GPa)</td>
<td>238</td>
<td>3.63</td>
</tr>
<tr>
<td>$E_{22}$ (GPa)</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>$E_{33}$ (GPa)</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>$\nu_{12}$</td>
<td>0.23</td>
<td>0.34</td>
</tr>
<tr>
<td>$\nu_{23}$</td>
<td>0.33</td>
<td></td>
</tr>
<tr>
<td>$\nu_{31}$</td>
<td>0.03</td>
<td></td>
</tr>
<tr>
<td>$G_{12}$ (GPa)</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>$G_{23}$ (GPa)</td>
<td>7.2</td>
<td></td>
</tr>
<tr>
<td>$G_{31}$ (GPa)</td>
<td>24</td>
<td></td>
</tr>
</tbody>
</table>

Coefficients of Thermal Expansion

<table>
<thead>
<tr>
<th></th>
<th>Fibre (HTA)</th>
<th>Matrix (6376)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{11}$ (K$^{-1}$)</td>
<td>$-0.1 \times 10^{-6}$</td>
<td>$54 \times 10^{-6}$</td>
</tr>
<tr>
<td>$\alpha_{22}$ (K$^{-1}$)</td>
<td>$10 \times 10^{-6}$</td>
<td></td>
</tr>
<tr>
<td>$\alpha_{33}$ (K$^{-1}$)</td>
<td>$10 \times 10^{-6}$</td>
<td></td>
</tr>
</tbody>
</table>

6376 Matrix

The 6376 epoxy matrix is assumed to be an elastic-plastic solid whose thermoelastic constants are also contained in Table 4.1. The yielding behaviour of the matrix phase is sensitive to the hydrostatic stress and as a result the Mohr-Coulomb yield criterion is employed. The Mohr-Coulomb criterion states that yielding will occur on a given plane when the shear stress ($\tau$) exceeds the cohesive stress of the material plus the frictional force acting along the failure plane, such that,

$$\tau = c - \sigma_n \tan \phi$$  \hspace{1cm} (4.1)

where $c$ is the cohesion yield stress, $\sigma_n$ is the normal stress acting on the failure plane and $\phi$ is the angle of internal friction. In Mohr’s stress plane ($\sigma - \tau$), the yield surface of the Mohr-Coulomb model can be expressed in terms of the maximum and minimum principal stresses such that,

$$f(\sigma_1, \sigma_3) = (\sigma_1 - \sigma_3) + (\sigma_1 + \sigma_3) \sin \phi - 2c \cos \phi = 0$$ \hspace{1cm} (4.2)

where $\sigma_1$ and $\sigma_3$ are the maximum and minimum principal stresses, respectively.
For the Mohr-Coulomb model, the cohesion stress and the angle of internal friction can be related to the tensile ($\sigma_T$) and compressive ($\sigma_C$) strengths of the material by the following expressions,

\[
\sigma_T = 2c \frac{\cos \phi}{1 + \sin \phi} \quad (4.3)
\]
\[
\sigma_C = 2c \frac{\cos \phi}{1 - \sin \phi} \quad (4.4)
\]

By combining Eqs. 4.3 and 4.4, the internal friction angle may be expressed in terms of the tensile and compressive strengths of the material,

\[
\phi = \sin^{-1} \left( \frac{\sigma_C - 1}{\sigma_C + 1} \right) \quad (4.5)
\]

Fiedler et al. (2005b) characterised the bulk mechanical behaviour of the 6376 epoxy matrix and determined that the tensile and compressive strengths were $\sigma_T = 103$ MPa and $\sigma_C = 264$ MPa, respectively (note: these are not the in-situ properties of the epoxy matrix). Using this data, together with Eqs. 4.3-4.5, the internal friction angle and cohesion stress for the 6376 epoxy matrix are found to be $\phi = 26^\circ$ and $c = 82$ MPa, respectively. As was carried out by González & Llorca (2007), a non-associative flow rule is used to compute the direction of plastic flow in which the dilatant angle is assumed to be zero. The flow potential ($G$) proposed by Menetrey & William (1995) is used which represents a smooth ellipse in the deviatoric stress plane may be expressed as,

\[
G = \frac{4(1 - e^2) \cos^2 \Theta + (2e - 1)^2}{2(1 - e^2) \cos \Theta + (2e - 1)\sqrt{4(1 - e^2) \cos^2 \Theta + 5e^2 - 4e}} \times \frac{3 - \sin \phi}{6 \cos \phi} \quad (4.6)
\]

in which $e$ and $\Theta$ may be determined using the following relationships,

\[
e = \frac{3 - \sin \phi}{3 + \sin \phi} \quad (4.7)
\]
\[
\Theta = \frac{1}{3} \arccos \left( \frac{J_3}{J_2} \right)^{3} \quad (4.8)
\]
where $J_2$ and $J_3$ are the second and third invariants of the deviatoric stress tensor. This non-associative flow rule is continuous and smooth along all directions meaning it does not contain singularities, unlike those present in the traditional Mohr-Coulomb yield surface (i.e. at the apex and edges of pyramidal surfaces shown in Fig. 2.17 (a)), allowing for efficient computational implementation.

**Fibre-Matrix Interface**

The behaviour of the fibre-matrix interface was modelled using cohesive elements available in ABAQUS. These elements were placed in a discrete region of negligible thickness ($10^{-4}$ µm) between the fibre and matrix phases. Their constitutive response was defined in terms of a traction-separation law which relates the separation displacement between the top and bottom faces of the element to the traction vector acting upon it. Figure 4.3 shows the bi-linear traction separation law which governs interfacial fracture, where $K^o$ is the initial elastic stiffness, $t^o$ is the cohesive interface strength and $\delta_m^o$ is the critical separation displacement. A very high initial elastic stiffness of $K^o = 10^5$ GPa/m was used to ensure the displacement continuity at the interface in the absence of damage. The initial linear response is followed by the initiation of damage, based on the maximum stress criterion, which is followed by linear softening. Failure of the fibre-matrix interface initiates when either the normal stress ($t_n$) or the shear stress ($t_s$) exceed the pre-defined normal ($t_n^o$) or shear ($t_s^o$) strengths according to,

$$\max \left\{ \frac{t_n}{t_n^o}, \frac{t_s}{t_s^o} \right\} = 1$$

(4.9)
Once either the critical normal or shear stresses are exceeded, softening at the interface occurs which can be described in terms of the scalar damage variable, $D$, where, $0 \leq D \leq 1$. The damage variable has an initial value of 0 which represents an undamaged interface. After the initiation of damage, $D$ evolves to a final value of 1 which represents a completely failed interface. The stress components of the cohesive element are described in terms of this damage variable by the following expressions,

$$ t_n = \begin{cases} (1-D)t_n & t_n \geq 0 \\ \frac{t_n}{t_n} & t_n < 0 \end{cases} $$  \hspace{1cm} (4.10)

$$ t_s = (1-D)t_s $$  \hspace{1cm} (4.11)

where $t_n$ and $t_s$ are the stresses predicted by the initial elastic stiffness for the current separation displacement assuming no damage such that,

$$ t_n = K_n^0 \delta_n $$  \hspace{1cm} (4.12)

$$ t_s = K_s^0 \delta_s $$  \hspace{1cm} (4.13)

To describe the evolution of damage under a combination of both normal and shear displacement, the effective displacement ($\delta^e$) may be defined as,
Transverse Tensile Damage Behaviour

\[ \delta_m = \sqrt{\delta_n^2 + \delta_s^2} \]  \hspace{1cm} (4.14)

where \( \delta_n \) and \( \delta_s \) are the normal and shear displacements, respectively. For linear softening, the damage parameter may then be defined as,

\[ D = \frac{\delta_m^f (\delta_m^{\text{max}} - \delta_m^o)}{\delta_m^{\text{max}} (\delta_m^f - \delta_m^o)} \]  \hspace{1cm} (4.15)

where \( \delta_m^{\text{max}} \) is the maximum effective separation displacement over the entire loading history, \( \delta_m^o \) is the effective displacement at the onset of damage (i.e. \( D = 0 \)) and \( \delta_m^f \) is the effective displacement for a completely failed interface (i.e. \( D = 1 \)). For a monotonic increasing load, \( \delta_m^{\text{max}} = \delta_m^o \) meaning the damage parameter, \( D \), increases as the separation displacement, \( \delta_m \), increases. During unloading \( \delta_m^{\text{max}} \) remains constant and consequently so does \( D \), meaning the stress decreases linearly with a slope \( K \) as the separation displacement, \( \delta_m \), decreases, as shown in Fig. 4.3.

This effective displacement at failure (\( \delta_m^f \)) determines the rate of damage in the element and this was defined in terms of the fracture energy which corresponds to the area under the traction separation curve, such that,

\[ \Gamma = \frac{1}{2} (t^o)(\delta_m^f) \]  \hspace{1cm} (4.16)

Due to the lack of experimental data available on the failure behaviour of the fibre-matrix interface, it has been assumed for this analysis that the interfacial normal strength was equal to the interfacial shear strength, i.e. \( t_n^o = t_s^o \), and the fracture energies were the same for Mode I and Mode II type failures, i.e. \( \Gamma_I = \Gamma_{II} \) (a similar assumption has previously been made by González & Llorca (2007a), Totry et al. (2008a), Canal et al. (2009), Kushch et al. (2010)).

The implicit implementation of material models undergoing softening behaviour can lead to sever convergence difficulties. In order to overcome convergence issues, a delayed damage approach was used by implementing viscous regularisation for the cohesive sections (Gao & Bower 2004). This means that ABAQUS allows the stresses to fall outside the limits set by the traction-separation laws governing behaviour at the
fibre-matrix interface. This evolution of the viscous stiffness degradation variable can be defined as follows,

\[
\dot{D}_v = \frac{1}{\mu} (D - D_v)
\]

(4.17)

where \( \mu \) is the viscosity parameter which represents the relaxation time of the viscous system and \( D_v \) is the regularised damage variable. For the current analysis the viscosity parameter was chosen to be \( \mu = 2 \times 10^{-4} \) (Keane 2009). This value was deemed suitable following a sensitivity analysis carried out, the details of which are contained in Appendix A.

4.3 Results

4.3.1 Microscopic Stress State after Thermal Cool-Down

The local stress state in the micromechanical models was examined following the cooling of the material from cure temperature (448 K) to room temperature (298 K). Figure 4.4 shows the distribution of the Interfacial Normal Stress (INS) around each fibre following the thermal cool-down from cure temperature. During the cooling phase, both the fibre and matrix phases undergo thermal contraction. Due to the mismatch in thermal expansion coefficients, the matrix experiences greater thermal strain than the fibres, causing significant compressive stresses to develop at fibre-matrix interfaces. The magnitude of the compressive stress is highly dependant on the local fibre arrangement surrounding the interface. This is highlighted for two regions in Fig. 4.4, in which there is a compressive stress of -94 MPa acting at the Point A, where the inter-fibre spacing measures only 0.32 \( \mu \)m. Meanwhile, the compressive stress acting at the Point B is significantly less, measuring only -34 MPa, while the inter-fibre distance at that location is much larger, measuring 0.74 \( \mu \)m. The same trends were observed throughout the RVE, where the magnitude of the compressive INS between neighbouring fibres increased as the inter-fibre spacing decreased, as was also found by Hojo et al. (2009).
Figure 4.4: Interfacial Normal Stress (INS) following the thermal cool-down from cure temperature.

Figure 4.5 shows the distribution of Interfacial Shear Stress (ISS) following the thermal cool-down from cure temperature. As was the case with the INS, the magnitude of the ISS between neighbouring fibres was found to increase as the inter-fibre spacing decreased. This is highlighted for two regions in Fig. 4.5, in which there is an ISS of +35 MPa acting at the Point A, where the inter-fibre spacing measures only 0.32 µm. However at the Point B, the ISS is almost half that, being +19 MPa, while the corresponding inter-fibre distance measures 0.74 µm. In Fig. 4.4, the position of the maximum compressive INS was centrally located directly between two closely neighbouring fibres. As can be seen in Fig. 4.5, the position of the maximum (and minimum) ISS is offset either side of this central location, towards the matrix rich region, as indicated at the Point A. Previous studies have shown that the presence of thermal residual stress at the interface can significantly affect mechanical behaviour. The compressive INS has been shown to be beneficial upon mechanical transverse loading (Hojo et al. 2009), while the ISS may contribute to the early onset of damage during the cooling phase (Gentz et al. 2004). These effects will be examined in the following section.
4.3.2 Fibre-Matrix Debonding

Effect of Interface Strength

The influence of fibre-matrix debonding on the transverse fracture behaviour was examined using a cohesive zone model at the fibre-matrix interface. The normal ($t_n^o$) and shear ($t_s^o$) strengths of the interface elements were varied to predict behaviour for a range of fibre-matrix interfacial strengths. Damage evolution at the interface was controlled by the interfacial fracture energy, $\Gamma$. For the present analysis, it will be initially assumed that the interfacial fracture energy is 10 $J/m^2$ (Varna et al. 1997). While this relatively low interfacial fracture energy represents rather brittle behaviour of the fibre-matrix interface, the largely linear transverse response to failure of the HTA/6376 material (O’Higgins et al. 2009), shown in Fig. 4.6, does indeed suggest this type of behaviour at the fibre-matrix interface. Shown also in Fig. 4.6 are the response curves of an RVE with a range of interfacial strengths for both the Mechanical Loading (ML) case and the Thermo-Mechanical Loading (TML) case. It is obvious that the interfacial strength has a significant effect on the macroscopic response of the RVE, with a higher transverse strength being seen for increasing fibre-matrix interfacial strength for the ML and TML cases. This section examines in detail the transverse damage behaviour for $t_n^o = 15$ MPa and $t_n^o = 60$ MPa for both the ML and TML cases. For completeness, the macroscopic response curves of the RVE with interface strengths of $t_n^o = 30$ MPa and $t_n^o = 90$ MPa have also been shown in Fig. 4.6.
For a weak interface ($t_{int}^o = 15$ MPa), shown in Fig. 4.6, the transverse strength is lowest and non-linear behaviour is observed at a relatively low strain level. At this interface strength, the TML case shows non-linear behaviour occurring earlier in the loading history than the ML case. During the thermal cool-down from cure temperature, some shear damage occurred at interfaces which were in close proximity to one another. Figure 4.7 (a) shows the density of cohesive elements in one RVE which had undergone shear damage as a result of the thermal cool-down from cure temperature (a deformation scale factor of 20 was used to highlight these damaged cohesive elements). Figure 4.7 (b) highlights one of these regions where fibre-matrix debonding occurred for two closely neighbouring fibres. Interfacial cracks initiated around both fibres in locations which were offset either side from the central region between the neighbouring fibres, as the analysis in the previous section suggested (i.e. the same locations to those shown in Fig. 4.5). As the temperature decreased, the interfacial cracks propagated away from the neighbouring fibre and towards a matrix rich region. This type of interfacial crack was typical of the type of damage observed in all the RVEs analysed and it also shows good agreement with experimental observations by Gentz et al. (2004), highlighted by the Region C in Fig. 4.8.

Figure 4.6: Transverse fracture behaviour of an RVE generated by the NNA for various interfacial strengths (Experimental results from O’Higgins et al. (2009)).
Figure 4.7: (a) Damaged cohesive elements following the thermal cool-down in an RVE with a weak fibre-matrix interface (b) Initiation and propagation of interface cracks due to thermal residual stress (Note: a deformation scale factor of 20 has been used in the above images).

Figure 4.8: Interfacial damage due to thermal residual stress (from Gentz et al. (2004)).

For some of the RVEs analysed at this interfacial strength ($t_{n/s} = 15$ MPa), the existence of these interfacial imperfections prior to mechanical loading, combined with the presence of thermal residual stress were enough to change the location where...
damage initiated and indeed the final fracture path observed, upon the application of a mechanical load. Figures 4.9 (a) and (b) show the progression of damage through an RVE for the ML and TML cases, respectively. The number at the top left of each RVE refers to the point in the loading history which that deformation plot represents; this point is identified in the response curves for the relevant loading case shown in Fig. 4.9 (c). In both the ML and TML cases, fibre-matrix debonding is widespread throughout the RVE, with interface cracks developing between closely neighbouring fibres which are aligned to the loading direction (i.e. Load Point 1 in Figs. 4.9 (a) and (b), i.e. the left-hand images). As the load increases, bands of interfacial cracks develop perpendicular to the loading direction. Within these bands of interfacial cracks, the intermediate matrix regions undergo yielding which allows the coalescence of neighbouring interfacial cracks. Finally, a band of interfacial cracks dominate to form the final fracture path across the RVE, which is perpendicular to the loading direction (i.e. Load Point 2 in Figs. 4.9 (a) and (b), i.e. the right-hand images), causing a drop in the stress-strain response, as shown by the Load Points 2 in Fig. 4.9 (c). Due to the relatively low interfacial strength (compared to the yield stress of the matrix), failure was dominated by fibre-matrix debonding and very little matrix yielding was evident (only in the bridged regions between interfacial cracks). Importantly, Figs. 4.9 (a) and (b) show vastly different fracture patterns for the ML and TML cases, respectively, highlighting the important influence thermal residual stress has on the onset and evolution of microscale damage. It should be noted that some of the pre-existing cracks from the thermal loading phase form the final fracture path in the TML case, as shown in Fig. 4.9 (b), suggesting that damage occurring during the cool-down from cure temperature significantly affects the crack location. However, the macroscopic response (shown in Fig. 4.9 (c)) only shows marginal differences between the ML and TML cases.
For an interfacial strength of $t_{int}^t = 60$ MPa, the TML case shows a higher transverse strength than the ML case, as shown in Fig. 4.10 (c). At this interfacial strength, no interfacial damage was observed as a result of the thermal cool-down from cure temperature. This increase in transverse strength is a result of the compressive INS
which developed as a result of the thermal cool-down from cure temperature, discussed in Section 4.3.1. In order for interfacial debonding to initiate, these significant residual compressive stresses (in the order of -100 MPa at some locations) acting at the interface must first be overcome upon mechanical transverse loading. This essentially increases the fibre pull-out energy required and as a result the onset of debonding for the TML case is delayed, such that the point at which non-linearity occurs (i.e. when debonding initiates in the RVE) in the TML response curve is 68% higher than the ML response curve, as shown in Fig. 4.10 (c). However, this large difference translates to only a 7.7% increase in transverse strength for the TML case. Figures 4.10 (a) and (b) show the progression of damage through the RVE for the ML and TML cases, respectively, with an interface strength of 60 MPa. Here fibre-matrix debonding is not as widespread as the previous interface strength examined (i.e. $t_{\text{int}}^{\alpha} = 15$ MPa), only initiating in a small number of locations ((i.e. Load Point 1 in Figs. 4.10 (a) and (b)) and as interfacial cracks grow, a dominant crack band and final fracture path forms (i.e. Load Points 2 in Figs. 4.10 (a) and (b)). Also, as the interfacial strength begins to approach the cohesion stress of the matrix, matrix yielding becomes more prevalent, as shown in Fig. 4.10 (b). This is seen in particular at a debonding interface, which is as a result of the stress concentration at the interface crack tip. Damage progression for the TML case, as seen in Fig. 4.10 (b), shows a slightly different fracture path than the ML case, which is a result of the presence of thermal residual stress caused by the cooling phase. It should be noted that when comparing the results from both interface strengths considered (i.e. $t_{\text{int}}^{\alpha} = 15$ MPa and $t_{\text{int}}^{\alpha} = 60$ MPa), the response curve of $t_{\text{int}}^{\alpha} = 15$ MPa, shown in Fig. 4.6, appears to be more ductile than the response curve of $t_{\text{int}}^{\alpha} = 60$ MPa. This difference in response can be attributed to the fact that the fracture energy for both cases considered did not change (i.e. $\Gamma = 10$ J/m$^2$). This means that for the weak fibre-matrix interface, the cohesive displacement at failure ($\delta_{m}^{f}$) is four times greater than for the strong fibre-matrix interface. This can be seen in Fig. 4.3 where, once the fracture energy is constant, any change to the maximum stress ($t^0$) will accordingly cause a change in the displacement at failure ($\delta_{m}^{f}$), as the area under the traction-separation curve must remain the same.
Figure 4.10: Progression of damage through an RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 60MPa (Note: a deformation scale factor of 5 has been used in the above images).

While Fig. 4.10 only shows a subtle difference between the final fracture paths for both the ML and TML cases for an interfacial strength of $\tau_{\text{int}}^{\ast} \approx 60$ MPa, some of the other RVEs analysed showed completely different fracture patterns. An example of one
of these RVEs is shown in Fig. 4.11 where, due to the altered microscopic stress state following the thermal load, the observed fracture paths for the ML and TML cases are dissimilar. The images shown in Fig. 4.11 correspond to similar Load Points as to those presented in Fig. 4.10.

![Progression of damage through another RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case.](image)

Figure 4.11: Progression of damage through another RVE with an interfacial strength of 60MPa for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case (Note: a deformation scale factor of 5 has been used in the above images).

It should also be noted that the sequence of damage predicted by the micromechanical models is very similar to that shown in Fig. 4.1, which was observed by Hobbiebrunken et al. (2006) in a carbon fibre/epoxy composite. For example, in Figures 4.9 (a) and (b) it is seen that debonding is widespread throughout the RVE, initiating in a number of locations between neighbouring fibres with a small inter-fibre spacing. These interfacial cracks grow and small regions of the matrix ‘bridge’ the debonded fibres. Upon further loading, intense yielding of the intermediate matrix
regions occurs allowing the interfacial cracks to coalesce, resulting in final fracture. The final fracture patterns for many of these micromechanical models (see Figs. 4.9-4.11) shows distinct similarities to that observed by Hobbiebrunken et al. (2006), shown in Fig. 4.1.

**Effect of Interface Fracture Energy**

The influence of interfacial fracture energy on the transverse deformation of the material was also examined. Three further interfacial fracture energies were considered which represent behaviour of a more brittle interface where, $\Gamma = 2.5 \text{ J/m}^2$ and also a more ductile interfaces where, $\Gamma = 25 \text{ J/m}^2$ and $\Gamma = 100 \text{ J/m}^2$. Figure 4.12 shows the transverse response of an RVE which had an interfacial strength of $t_{\text{int}} = 60$ MPa for a range of interfacial fracture energies. Firstly, non-linear behaviour is observed at the same point in the loading history for all fracture energies considered, as the interface strength is the same for all cases. However, for an interfacial fracture energy of $\Gamma = 2.5 \text{ J/m}^2$, there is a reduction in the transverse strength in both the ML and TML cases, due to the increased rate of softening at the interface. This causes more aggressive stress redistribution in regions adjacent to interfacial cracks and results in a macroscopic brittle response with a sudden stress drop after the peak load is reached. An increase in fracture energy to $\Gamma = 25 \text{ J/m}^2$ causes a more ductile macroscopic response of the material and ultimately increases the transverse strength for both the ML and TML cases. A further increase in fracture energy to $\Gamma = 100 \text{ J/m}^2$ has a similar effect on the macroscopic response of the composite. It is noticeable that for higher fracture energies the effect of thermal residual stress appears to be less. For a brittle interface (i.e. $\Gamma = 2.5 \text{ J/m}^2$), the difference in transverse strength between the ML and TML cases was 8.9% while for a ductile interface (i.e. $\Gamma = 100 \text{ J/m}^2$) the difference was only 0.6%. Thus, it was found here that the slower rate of damage progression for ductile interfaces almost negates the effects of thermal residual stress.

More importantly, the effect of increasing the fracture energy has been to increase the strain to failure of the composite. This has important implications as it is the low strain to failure of transverse plies which causes damage to initiate in cross-ply laminates (Gamstedt & Sjögren 1999). Through the process of damage accumulation, micro-cracks in these transverse plies cause other damage mechanisms to evolve, such as inter-laminar delamination or even fibre fracture in neighbouring plies. Indeed many
of the recent research efforts into fibre surface treatments are concerned with introducing a softer, more ductile interface in order to improve the strain to failure of transverse plies (Benzarti et al. 2001). These findings substantiate many of these research efforts by highlighting that a more ductile fibre-matrix interface inhibits the development of transverse cracks.

![Graph showing effect of interfacial fracture energy on transverse response](image)

Figure 4.12: Effect of interfacial fracture energy on transverse response (Experimental results from O’Higgins et al. (2009)).

### 4.3.3 Damage Accumulation under Cyclic Loading

Composite laminates exhibit a sequential accumulation of a multitude of hierarchical dissipative mechanisms whose initiation and subsequent propagation depends heavily upon the loading history. These dissipative mechanisms occurring at the constituent level, such as dislocations, micro-cracks/voids and interface decohesions, are responsible for macroscopic non-linear material behaviour. Figure 4.13 (a) shows the experimental response of the HTA/6376 material under a transverse tensile cyclic loading regime. Three loading cycles are shown, where the material is loaded to the Point A, unloaded to zero stress, reloaded to the point B, unloaded to zero stress, reloaded to the Point C and finally unloaded to zero stress. The non-linear material behaviour can be attributed to two distinct mechanical processes, that is material plasticity (slips and dislocations) and material damage (nucleation of micro-cracks and voids). Here, plasticity is manifested in the response as the emergence of
permanent plastic strains, which is shown in Fig 4.13 (a) as $\varepsilon_{22}^p$, while material damage is characterised by stiffness loss or change in the elastic modulus of successive loading cycles, i.e. the difference between $E_{22}^0$ on the first loading cycle and $E_{22}^i$ on any successive loading cycle. Figure 4.13 (b) shows the response of an RVE which has been subject to the same loading cycle as the experimental sample. Shown on the micromechanics curve are the same three loading cycle points as in Fig. 4.13 (a), i.e. Points A, B and C. Here, it is the TML case which is considered and the interfacial strength and fracture energy were assumed as $\tau_{n/s} = 90$ MPa and $\Gamma = 10$ J/m$^2$, respectively. While a direct correlation to the experimental curve is not evident, the same characteristics in the RVE response are observed. Non-linear behaviour exists upon loading of the RVE, while upon unloading the response shows both a loss in stiffness (due to damage) and a permanent plastic strain (due to plasticity).
To examine these characteristics in more detail, the RVE is subjected to a regime of successive transverse tensile and compressive loadings. This particular sequence is used to illustrate the accumulation of damage in the material and its effect on subsequent loading cycles. The RVE is first loaded to a tensile strain of 1%, followed by compressive loading to a strain of -2% and finally reloaded in tension to failure. Figure 4.14 shows the response of the material subject to the described loading sequence.
The initial transverse tensile load (Path O-A) shows non-linear behaviour as a result of fibre-matrix debonding and yielding in the matrix, which are shown for the Load Point A in the RVE insert in Fig. 4.14 (a). The unloading path of the material (Path A-B) shows a reduced slope denoting a loss in material stiffness caused by crack opening at fibre-matrix interfaces. Also, unloading does not take place through the origin (O) as some permanent plastic strain remains in the material. However, crack closure does occur at debonded interfaces during the unloading phase, as shown by the final configuration of the RVE at the Load Point B in the RVE insert in Fig. 4.14 (b). Upon subsequent compressive loading (Path B-C), the compressive modulus is recovered to almost that of the undamaged material as a result of crack closure and compressive load take up between the newly formed crack faces. Further non-linear behaviour in the compressive loading phase is seen as a result of more fibre-matrix debonding and matrix yielding occurring, as shown at the Load Point C in the RVE insert in Fig. 4.14 (c). A reduction in the compressive modulus is seen during the next unloading phase (Path C-D) as a result of damage which occurred during compressive loading. Again, unloading does not take place through the origin as a new permanent plastic strain exists in the material as a result of the previous loading cycles. Upon subsequent tensile loading (Path D-E), a further reduction in the tensile modulus is also seen (compared to the unloading phase in Path A-B) as a result of cracks developed during the previous compressive loading phase. It is also noticeable that the tensile strength for this cycle has reduced, which indicates that the material was at the cusp of its ultimate tensile strength at Load Point A. The compression damage sustained during the previous load cycle was enough to actually trigger ultimate failure (i.e. Load Point E) in the composite at a lower stress than at Load Point A.
The damage accumulation behaviour highlighted here shows the complex failure process which composite laminates undergo, especially when subject to multiple loading cycles and different stress states. The current state-of-the-art in continuum damage modelling of composite structures does not capture such a wide range of behaviour. The micromechanical model predicts stiffness reduction and permanent plastic strain in the material due to various loading regimes, all the while capturing the actual microscopic damage progression in each of the constituent phases of the composite.

4.4 Concluding Remarks

A comprehensive study has been carried out examining the transverse damage behaviour of a carbon fibre/epoxy composite. Using a micromechanics damage model...
the effects of fibre-matrix debonding, thermal residual stress and cyclic loading were analysed. The presence of thermal residual stress was found to alter the microscopic stress state significantly. It is effective in offsetting interfacial decohesion as a result of thermally induced compressive stresses acting at the fibre-matrix interface. These stresses compensate for subsequent tensile stresses developed under transverse tensile loading. Similar results reporting beneficial effects of thermal residual stress were also found by Maligno et al. (2008) and Hojo et al. (2009). However, if a weak fibre-matrix interface is present, the thermally induced stresses can have a detrimental effect causing interfacial cracks to develop during the cooling phase. The results from the micromechanical models highlight the influence of the manufacturing conditions on the overall fracture behaviour as the cure temperature will affect the magnitude of thermal residual stresses.

The properties of the fibre-matrix interface greatly influenced the transverse strength of the material, with the interfacial strength controlling the overall transverse strength. The interfacial toughness (or fracture energy) also has a significant effect on the fracture behaviour with increased ductility at the fibre-matrix interface increasing the ability of the material to resist fracture. This micromechanical model shows that tailoring the interface properties to a suitable level could potentially allow for the transverse failure strain to be increased, meaning the effects of transverse matrix cracking, and other resulting damage mechanisms, i.e. delamination at the transverse ply boundary, could be reduced.

The micromechanical model developed herein was found to produce similar failure patterns to those observed experimentally for similar composite material systems for both thermal (Gentz et al. 2004) and mechanical (Hobbiebrunken et al. 2006) loading. Under cyclic loading, the micromechanical model provided novel insight into the microscopic damage accumulation that forms prior to ultimate failure, and clearly highlighted the different roles that fibre-matrix debonding and matrix plasticity play in forming the macroscopic response of the composite. Such information is vital to the development of accurate continuum damage models, which often smear these effects using non-physical material parameters.
Chapter 5

Micromechanical Modelling of Transverse Shear Deformation in Fibre Reinforced Composites

5.1 Introduction

In this chapter, the behaviour of the carbon fibre/epoxy composite under transverse shear loading is examined. The interlaminar shear strength (ILSS) is an important property in laminate configurations, particularly under compressive or shear loading scenarios. Through the thickness reinforcement can improve the ILSS, however, current design practices do not allow for fibres to be aligned in the thickness direction of the material. In an attempt to improve the interlaminar shear behaviour and prevent delamination between plies, a number of techniques have been developed to reinforce the thickness direction of a laminate such as Z-pinning, stitching and the use of carbon nanotubes (Fan et al. 2008). While these techniques are effective in improving the ILSS, interlaminar shear failure has been shown to be highly dependant on the intra-ply properties such as fibre-matrix interfacial strength and resin formulation (Thomason 1995). Under transverse shear loading, Hinz et al. (2009) used in-situ SEM experiments to show that delamination, or interlaminar shear failure, was caused by the coalescence of intra-ply damage mechanisms. As fibre-matrix debonding was one of the primary damage mechanisms observed, as shown in Fig. 5.1, it was concluded that the
interlaminar shear strength of a laminate could be improved by changing the properties at the fibre-matrix interface.

![Figure 5.1: In-Situ SEM observation of fibre-matrix debonding due to a transverse shear load applied during a double notch shear test (from Hinz et al. (2009)).](image)

While Llorca, González and co-workers (Totry et al. 2008a, Canal et al. 2009) have shown the important influence fibre-matrix interfacial strength has on the transverse shear behaviour, the effects of many other intra-ply properties, such as interfacial toughness, local fibre distribution, fibre volume fraction and thermal residual stress, have not been examined, to date. In particular, it has been already shown in Chapter 4 that the presence of thermal residual stress has a marked effect on both the interfacial stress state and the propagation of local damage mechanisms for the transverse tensile loading case, suggesting it could significantly influence material behaviour under transverse shear loading. Thus, this chapter examines in detail the effects of thermal residual stress, in addition to the effects of fibre-matrix debonding and local fibre volume fraction, on the transverse shear behaviour in a number of multi-fibre statistically equivalent RVEs.

This chapter is organised as follows. In Section 5.2, the important details regarding the micromechanical modelling procedure are outlined. In Section 5.3, the stress state at the fibre-matrix interface is examined and the effect of the fibre-matrix interface properties on the transverse shear behaviour of the material is assessed. Section 5.4 summarises the main findings and provides some concluding remarks on the studies carried out in this chapter.
Note: The findings from Chapter 5 have been published as a peer-reviewed journal article in Composites Part A: Applied Science and Manufacturing, under the title *A Micromechanical Study on the Effect of Intra-Ply Properties on Transverse Shear Fracture in Fibre Reinforced Composites* (Vaughan and McCarthy 2011b).

5.2 Finite Element Modelling

In this chapter, three studies have been carried out to examine the transverse shear behaviour of the composite material.

1) A linear elastic analysis is carried out to examine the stress state at the fibre-matrix interface under a transverse shear strain of 1%. The effect of thermal residual stress on the microscopic stress state is also considered.

2) The effect of the fibre matrix-interface properties on the transverse shear behaviour of the material is examined using a cohesive zone model. Parameter studies are carried out examining the influence of interfacial strength, interfacial toughness (fracture energy) and local fibre volume fraction on material behaviour.

3) Finally, using a combined transverse normal and shear loading regime, the effect of thermal residual stress on the transverse fracture surface (in the $\sigma_{22} - \tau_{23}$ stress space) is determined.

5.2.1 Generation of Micromechanical Models

As was carried out in Chapter 4, the Nearest Neighbour Algorithm (NNA) has been used to generate five separate RVEs, each statistically similar but topologically different to that shown in Fig. 5.2 (a). These measured 66×66 µm ($\delta = 20$) and contained approximately 80 fibres. Python scripts were used to create finite element models of the RVEs in the ABAQUS finite element code. The fibre and matrix regions were discretised using a quad-dominated mesh which consisted of predominantly 4-noded (CPEG4) and a relatively small number of 3-noded (CPEG3) full integration generalised plane strain elements, assuming a small strain formulation. The periodic boundary conditions, which were described in Chapter 3, were again applied to the micromechanical models and two load cases are also considered here. The first being a
mechanical transverse shear load imposed on the RVE by applying a horizontal displacement ($\delta_s/2$) to the active control node, $n_4$, together with a complimentary vertical displacement ($\delta_v/2$) to the active control node, $n_2$, as shown in Fig. 5.2 (a). This is referred to throughout as the Mechanical Loading (ML) case. The second load case considers the effects of thermal residual stresses in the micromechanical models, whereby a thermal load is invoked where a temperature change, $\Delta T = -150$ K, is applied globally to each node in the model, as shown in Fig. 5.2 (b), and this is subsequently followed by a mechanical transverse shear load, identical to that shown in Fig. 5.2 (a). This is referred to throughout as the Thermo-Mechanical Loading (TML) case.

![Figure 5.2](image)

**Figure 5.2:** Periodic boundary conditions applied to RVE to simulate transverse shear loading for the (a) Mechanical Loading case and (b) Thermo-Mechanical Loading case.
5.2.2 Material Behaviour

The behaviour of the constituent materials is the same as that described in Chapter 4. Thus, the HTA fibres are assumed to be linear elastic while the 6376 matrix behaves as an elastic-plastic solid where yielding behaviour is described by Mohr-Coulomb plasticity theory, whose constants are given in Table 5.1. The behaviour of the fibre-matrix interface is the same as was outlined in Chapter 4, where failure is governed by a bi-linear traction-separation law based on the maximum stress criterion. Again, it was assumed in this analysis that the interfacial normal strength was equal to the interfacial shear strength, i.e. $t_{n}^0 = t_{t}^0$, and the fracture energies were the same for Mode I and Mode II type failure.

Table 5.1: Mohr-Coulomb Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Matrix (6376)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$ (MPa)</td>
<td>82</td>
</tr>
<tr>
<td>$\phi$</td>
<td>26°</td>
</tr>
</tbody>
</table>

5.3 Results

5.3.1 Interfacial Stress State under Transverse Shear Loading

A macroscopic transverse shear strain of 1% was applied to the RVE shown in Fig. 5.2 (a) to examine the local microscopic stress state at the fibre-matrix interface, while the composite remained in the elastic loading regime. Figure 5.3 shows the deformation of the RVE under mechanical transverse shear loading. To analyse the effect of thermal residual stress on the local microscopic stress state, the interfacial stress distribution around two isolated fibres have been examined. These are highlighted in Fig. 5.3 as Fibre $A_0$ and Fibre $B_0$. The analysis considers both the Mechanical Loading (ML) and Thermo-Mechanical Loading (TML) cases. Also, the interfacial stress state has been examined following the Thermal Loading (TL) phase. Figures 5.4 (a) and (b) show the distribution of the Interfacial Normal Stress (INS) around Fibre $A_0$ and Fibre $B_0$, respectively, for each of the loading cases considered. In these figures, the fibre boundary corresponds to zero stress, i.e. any point on the distribution which lies outside the fibre boundary corresponds to a tensile INS, while any point of the distribution which lies inside the fibre boundary corresponds to a compressive INS.
Transverse Shear Damage Behaviour

Figure 5.3: Transverse shear deformation of an RVE showing directions of the maximum ($\sigma_1$) and minimum ($\sigma_3$) principal stresses.

Figure 5.4 (a) shows the distribution of INS around Fibre $A_0$. For the ML case, there are two distinct positive peaks in the INS which occur at opposite sides of the fibre. These local maxima of 32 MPa and 26 MPa occur at these locations as they are aligned with the maximum principal tensile loading axis of the RVE under a transverse shear load. This is shown by $\sigma_1$ in Fig. 5.3 which is inclined at an angle $\theta = +45^\circ$ and $\theta = -135^\circ$ to the horizontal shear loading axis (i.e. the 2-axis). The magnitude of the INS at these locations is relatively low compared to the macroscopic shear stress applied which, for a 1% transverse shear strain, was $\tau_{33} = 36.9$ MPa. Meanwhile, the two lowest points on the distribution of the INS also occur on opposite edges of the fibre and have magnitudes of -71 MPa and -85 MPa. These local minima occur close to the direction of the minimum (compressive) principal loading axis, which makes an angle of $\theta = -45^\circ$ and $\theta = +135^\circ$ to the horizontal shear loading axis (i.e. the 2-axis), as shown by $\sigma_3$ in Fig. 5.3. Here, the INS is influenced by the close proximity of the neighbouring fibres, Fibre $A_2$ and Fibre $A_4$, as the local minima are somewhat inclined towards these fibres. Figure 5.4 (b) shows the distribution of INS around Fibre $B_0$. Here, for the ML case, the peaks in the INS are no longer orientated along the maximum principal tensile loading axis, but instead are clearly orientated towards the neighbouring fibres, Fibre $B_1$ and Fibre $B_3$, and these have magnitudes of 67 MPa and 89 MPa, respectively. These are much higher than the applied macroscopic shear stress ($\tau_{33} = 36.9$ MPa) which is a result of the small inter-fibre spacing between the fibres at these locations. Meanwhile, the minimum INS of -102 MPa almost coincides with the
orientation of the neighbouring fibre, Fibre $B_4$, which happens to be very close to the orientation of the minimum principal (compressive) loading axis ($\theta = -45^\circ$). Again, the high INS at this location is due to the small inter-fibre spacing between the two fibres. Thus, for transverse shear loading, stress is directed through the much stiffer fibres and their ability to transfer load depends on the proximity of their neighbouring fibres.

![Figure 5.4: Distribution of Interfacial Normal Stress around (a) Fibre $A_0$ and (b) Fibre $B_0$.](image)

For the TML case, the INS surrounding Fibre $B_0$ has been significantly altered by the thermal cure cycle, as shown in Fig. 5.4 (b). The magnitude of the local maxima in the distribution of the INS in some locations has been reduced significantly, i.e., near Fibre $B_1$ and Fibre $B_3$ the magnitude of the INS has been reduced to $17\%$ and $50\%$ of the original INS (following the ML load), respectively. Meanwhile, the magnitude of the minimum (compressive) INS has seen a significant increase, as shown near Fibre $B_4$, where the INS has increased to $179$ MPa which is a $75\%$ increase on the original INS. These significant changes are explained by the distribution of INS following the Thermal Loading (TL) phase, also shown in Fig. 5.4 (b). Due to the mismatch in thermal expansion coefficients of the constituent phases, the matrix phase undergoes significant thermal contraction causing large compressive stresses to develop at the fibre-matrix interface, as shown by local minima in the INS at orientations aligned with Fibres $B_1$, $B_2$, $B_3$ and $B_4$ in Fig. 5.4 (b). Again, the magnitude of these compressive INS increase as the fibre spacing decreases. Upon subsequent mechanical loading (i.e., the TML case) the compressive stresses must be overcome resulting in a lower maximum
INS around the fibres when compared to the ML only case, shown by the INS towards Fibre B₁ and Fibre B₃ in Fig. 5.4 (b). Similarly, the compressive INS developed during the TL phase contributes to the compressive INS developed upon subsequent mechanical loading for the TML case, resulting in larger compressive INS between neighbouring fibres than those in the ML only case, such as towards Fibre B₂ and Fibre B₄ in Fig. 5.4 (b). In fact, the resulting interfacial stress state in the TML case is almost a direct superposition of the interfacial stress state following the individual thermal loading and mechanical loading phases. Similar trends for the TML case can be observed for the distribution of INS around Fibre A₀, as shown in Fig. 5.4 (a).

The distributions of the Interfacial Shear Stress (ISS) around Fibre A₀ and Fibre B₀ are shown in Figs. 5.5 (a) and (b), respectively. For the ML case in both Figs. 5.5 (a) and (b), positive shear stresses develop near the fibre poles as these locations are parallel to the plane of the positive shear loading axes, which occurs at an angle \( \theta = +90^\circ \) and \( \theta = -90^\circ \). Meanwhile, negative shear stresses develop near the equators of the fibre, which coincide with the negative shear loading axes which are orientated at an angle \( \theta = 0^\circ \) and \( \theta = 180^\circ \). The influence of neighbouring fibres on the orientation of the max/min ISS is less pronounced than the previous case (discussed above) although the magnitude of the ISS is affected by the proximity of the neighbouring fibres. A clear example of this is the large ISS of +52 MPa which develops towards the Fibre A₃, shown in Fig. 5.5 (a), and also the large ISS of +50 MPa which develops towards the Fibre B₁, shown in Fig. 5.5 (b).

During the Thermal Loading (TL) phase, the magnitude of the ISS which develop, shown in Figs. 5.5 (a) and (b), are noticeably less than that of the compressive INS from the previous case (shown in Figs. 5.4 (a) and (b)). The largest ISS which develops around either fibre is +34 MPa which occurs around Fibre B₀ and is orientated towards the closely neighbouring fibre (Fibre B₄), as shown in Fig. 5.5 (b). However, these relatively small thermal residual (shear) stresses do affect the interfacial stress state upon subsequent mechanical loading (i.e., for the TML case). Again, there is a superposition of the thermal residual and mechanical stresses at the interface for the TML case. This means that at some locations on the interface the ISS is reduced, such as the local minima of -70 MPa and -67 MPa seen in Fibre A₀ (Fig. 5.5 (a)). Meanwhile, at other locations it is increased, in some cases significantly, such as the
new local maximum ISS around Fibre B_0 of +63 MPa, which occurs towards Fibre B_4 and represents a 46% increase in ISS at that location, as shown in Fig. 5.5 (b). Interestingly for the TML case, the ISS at some locations, such as towards Fibre B_4 in Fig. 5.5 (b), is now of similar magnitude to the INS which has been altered significantly by the presence of thermal residual stress, suggesting it could affect the onset and evolution of local damage processes.

![Figure 5.5: Distribution of Interfacial Shear Stress around (a) Fibre A_0 and (b) Fibre B_0.](image)

Figures 5.4 and 5.5 yield important information regarding both the effects of thermal residual stress and the effect of the local fibre distribution on the interfacial stress state under transverse shear loading. The effects of thermal residual stress found here are, in fact, very similar to those seen under transverse tensile loading (Hojo et al. 2009).

### 5.3.2 Fibre-Matrix Debonding

**Effect of Interface Strength**

This section discusses the influence of fibre-matrix debonding on transverse shear deformation which was examined using a cohesive zone model at the fibre-matrix interface. The normal (\( t_n^o \)) and shear (\( t_s^o \)) strengths of the interface layer were varied to predict behaviour of a range of fibre-matrix interfacial strengths. Damage evolution at the interface was controlled by the interfacial fracture energy, \( \Gamma \), which was chosen to
be $\Gamma = 10 \text{ J/m}^2$ (Varna et al. 1997). The effect of fibre-matrix interface strength on the transverse shear behaviour is shown in Fig. 5.6. It is obvious that the interfacial strength significantly affects the response of the RVE, with the failure strength of the composite increasing as the interfacial strength is increased, as might be expected.

![Graph](image)

Figure 5.6: Transverse shear behaviour of an RVE generated by the NNA for both the ML and TML cases for different interface strengths.

For an interfacial strength of $t_{n/s}^o = 15 \text{ MPa}$, the transverse shear strength is lowest and non-linear behaviour is seen in the TML case very early in the loading history, as shown in Fig. 5.6. As was found in Chapter 4, some interfacial cracks developed between closely neighbouring fibres during the thermal loading phase. Upon subsequent mechanical loading, these damaged interfaces cause some early non-linear behaviour for the TML case, however upon increased loading the transverse shear strength is similar to that of the ML case. Figures 5.7 (a) and (b) show the progression of damage through an RVE with an interfacial strength of $t_{n/s}^o = 15 \text{ MPa}$ for both ML and TML cases, where the number in the top left of each image corresponds to a particular Load Point in the stress-strain response curves, which are shown in Fig. 5.7 (c). The initial non-linear behaviour seen at Load Point 1 (Fig. 5.7 (c)) is a result of widespread fibre-matrix debonding. As the linear elastic analysis from the previous section suggests, fibre-matrix debonding initiates between numerous closely neighbouring fibres which are orientated at approximately $45^\circ$ to the 2-axis, as shown in Figs. 5.7 (a) and (b) (Load Point 1). Further non-linear behaviour is observed at Load
Point 2 (Fig. 5.7 (c)) as the damage propagates and neighbouring interface cracks begin to coalesce through shear yielding in the intermediate matrix regions, as shown in Fig. 5.7 (a) and (b) (Load Point 2). Final fracture occurs at Load Point 3 (Fig. 5.7 (c)) as a dominant band of interface cracks develop to form a final fracture path across the RVE, as shown in Fig. 5.7 (a) and (b) (Load Point 3). This fracture path is orientated approximately perpendicular to the main principal tensile loading axis (see Fig. 5.3). In some of the RVEs analysed, the progression of damage through the microstructure differed somewhat between the ML and TML cases, as a result of thermal residual stress formed during the TL phase. The observed differences, which in this case are minimal, between final fracture paths for the ML and TML cases for this RVE are shown in Figs. 5.7 (a) and (b) (at Load Point 3).
Figure 5.7: Progression of damage through an RVE with an interfacial strength of 15MPa for the (a) Mechanical Loading case (b) Thermo-Mechanical Loading case and (c) stress-strain response for an interfacial strength of 15MPa. (Note: a deformation scale factor of 2 has been used in the above images).

For an interfacial strength of $\tau_{int} = 60$ MPa, the ML case exhibits a slightly higher transverse shear strength than the TML case, as shown in Fig. 5.8 (c), which can
be attributed to the increase in the interfacial shear stress following the thermal loading phase, which was outlined in Fig. 5.5. Plots of the damage progression in an RVE for the ML and TML cases for this 60 MPa interface strength are shown in Figs. 5.8 (a) and (b), respectively. The non-linear behaviour at the Load Point 1 (see Fig. 5.8 (c)) is a result of fibre-matrix debonding developing between closely neighbouring fibres aligned along the main tensile loading direction (+45° to the horizontal shear loading axis). Fibre-matrix debonding is not widespread across the RVE, but is concentrated between a small number of neighbouring fibres, as shown in Figs. 5.8 (a) and (b) (Load Point 1). It is also noticeable that, due to the presence of thermal residual stress, the location at which damage initiates in the RVE is different for the ML and TML cases. At Load Point 2 (see Fig. 5.8 (c)) there has been a drop off in the stress-strain response curve, which is a result of interface cracks propagating to neighbouring fibres. This occurs due to stress redistribution from the initially debonded interfaces to adjacent neighbouring fibres which, in turn, cause interface cracks to develop at these fibres, as shown in Figs. 5.8 (a) and (b) (Load Point 2). Finally, at Load Point 3, damage propagates through the RVE to form a fracture path which is perpendicular to the direction of the main tensile loading axis. This fracture path is made up of a combination of interface cracks and intense plastic deformation of the small intermediate matrix regions, as shown in Figs. 5.8 (a) and (b) (Load Point 3). At Load Point 3, the final fracture paths in the RVE are different for the ML and TML cases, thus highlighting the effect of thermal residual stress on the local microscopic stress state. The debonding pattern predicted by the micromechanical model, shown in Figs. 5.8 (a) and (b), is similar to that observed by Hinz et al. (2009), who used experimental in-situ microscopy and found that, on occasion, a series of interface cracks in the intra-ply region coalesced to form a diagonal shear crack across the lamina.
For an interfacial strength of $\tau_{u,s} = 120$ MPa, the response of the ML case is largely similar to the TML case, as shown in Fig. 5.9 (b) As the interface strength is now larger than the matrix yield stress (i.e. $\sigma = 82$ MPa), failure of the material is now governed by the matrix behaviour. From the previous section it was seen that the TL phase caused a moderate increase (approximately 40% at some locations) in the
magnitude of the ISS. Although yielding in the matrix is largely dominated by the shear stress, this moderate change in the microscopic stress state due to thermal residual stress translates to an almost negligible change in the macroscopic behaviour. This is most likely due to the fact that the most significant shear stresses as a result of the TL phase develop only between closely neighbouring fibres, while the majority of matrix regions remain unaffected. As a result, the early onset of shear yielding for the TML case remains localised in these small inter-fibre regions and therefore the macroscopic response remains largely unaffected.

As the macroscopic stress-strain response in Fig. 5.9 (b) suggests, the deformation seen in all RVEs was almost identical for both the ML and TML cases for the 120 MPa interface strength and so, plots of deformation observed in the RVEs will only be shown for the ML case. Figure 5.9 (a) shows the onset and evolution of plastic deformation in the matrix phase in an RVE subject to transverse shear loading. Prior to the onset of plastic deformation in the matrix, the maximum local shear stress ($\tau_{23}$) occurs between two neighbouring fibres, whose inter-fibre spacing is only 0.23 µm, as indicated in Fig. 5.9 (a). These neighbouring fibres are orientated parallel to the horizontal shear loading axis. At Load Point 1 in Fig. 5.9 (a), shear yielding of the matrix has taken place between these fibres and indeed at other locations throughout the RVE, which have a similar fibre arrangement, i.e. where neighbouring fibres are in close proximity to one another and are orientated parallel to either the horizontal or vertical shear loading axes. The yielding behaviour at these locations is responsible for the initiation of non-linear behaviour in the macroscopic response, as indicated by the corresponding Load Point 1 in Fig 5.9 (b). From some (not all) of these locally yielded regions, shear bands propagated across the RVE, as shown in Fig. 5.9 (a) (Load Point 2), resulting in further non-linear behaviour, as shown in Fig. 5.9 (b) at the corresponding Load Point 2. The shear bands propagated into what can be described as matrix rich paths which were unobstructed by fibres and were oriented almost parallel to both the horizontal and vertical shear loading axes (theoretically, the Mohr-Coulomb model predicts that under pure shear, plastic yielding will occur on a plane inclined at an angle of $\phi/2$ to the applied shear loading axis). These slip paths cause very high shear stresses to develop in some regions of the RVE, particularly for fibres in the path of the shear band. The large shear stresses for the highlighted fibres in Region A, shown in Fig. 5.9 (a), eventually cause debonding to occur between these closely
neighbouring fibres at the Load Point 3, resulting in a drop-off in stress in the overall response, as shown in Fig. 5.9 (b) (Load Point 3). Thus, the final fracture path is made up of a combination of heavily yielded matrix regions, together with a number of interfacial cracks brought about by high shear stresses. Totry et al. (2008a) observed similar fracture paths in relation to weak/strong fibre-matrix interfaces under transverse shear loading as also observed here between the $t_{int}^{\alpha} = 60$ MPa and $t_{int}^{\alpha} = 120$ MPa cases.

![Figure 5.9](image)

Figure 5.9: (a) Progression of damage through an RVE with an interfacial strength of 120 MPa for the Mechanical Loading case and (b) stress-strain response for an interfacial strength of 120 MPa (Note: a deformation scale factor of 2 has been used in the above images).

It is also interesting to observe the local damage progression in the Region B in Fig. 5.9 (a). At Load Point 1, unlike the Region A, the interface fails by a crack opening due to the interfacial normal stress being exceeded and this fracture is aligned close to the main tensile loading axis of the RVE, in a similar fashion to the previous interface.
strengths examined (i.e. $t_{n/s}^o = 15$ MPa and $t_{n/s}^o = 60$ MPa). As the fibre-matrix bond fractures, the shear load is taken up by the matrix region immediately adjoining the interfacial crack resulting in plastic deformation in this region. This sequence of damage is in contrast to that at the Point A, where initial matrix yielding subsequently led to fibre-matrix debonding, even though the parameters governing behaviour of the matrix and fibre-matrix interface at both locations were identical. This highlights the outstanding influence the local fibre distribution has on the onset and evolution of damage within the microstructure and indeed the complexity of the failure process in fibre reinforced composites due to the number of competing damage mechanisms involved.

**Effect of Local Fibre Volume Fraction**

At Load Point 2 in Fig. 5.9 (a), it was observed that shear bands propagated into matrix rich paths due to the lack of reinforcement in these regions. The formation of shear bands in these resin rich paths suggests that in a given transverse ply the resin rich region at the ply boundary, which tends to have a lower fibre volume fraction (locally) than the rest of the lamina, would be highly susceptible to shear yielding as a result of a transverse shear load. To examine this in more detail, an additional RVE was generated using the NNA, which included a matrix rich region at the top and bottom boundaries, as shown in Fig. 5.11 (a). This was implemented by changing the NNA so as not to allow any fibres to penetrate the top and bottom edges of the RVE, in a similar fashion to a transverse ply boundary in a laminate. The effect of fibre-matrix interface strength for this matrix rich RVE on the transverse shear behaviour is shown in Fig. 5.10.
Transverse Shear Damage Behaviour

Figure 5.10: Effect of interface strength on transverse shear behaviour of a ‘matrix rich’ RVE.

This matrix rich RVE, which is shown in Fig. 5.11 (a), illustrates how the inter-ply region is subject to large shear deformations due to the lack of reinforcement at these locations. For an interfacial strength of \( t_{\phi/\theta}^0 = 120 \) MPa, the initial non-linear behaviour observed at the Load Point 1 of this matrix rich RVE, as shown in Fig. 5.11 (b), is similar to the previous unmodified RVE analysed, shown in Fig. 5.9 (b). This is a result of shear yielding between closely neighbouring fibres which are parallel to either the horizontal or vertical shear loading axes, such as those shown in Fig 5.11 (a) (Load Point 1). However, upon further loading of this matrix rich RVE, yielding in these regions remains localised (does not propagate) as a result of the reinforcing effect of surrounding fibres. The further non-linear behaviour observed at the Load Point 2, shown in Fig. 5.11 (b), is a result of shear deformation which takes place in the matrix rich path at the top and bottom edges of the RVE, as shown in Fig. 5.11 (a), even though no stress concentrations are visible in this region. At the Load Point 3, shown in Fig. 5.11 (b), an intense yield path has formed in the region, as shown in Fig. 5.11 (a) (Load Point 3), and very little interfacial damage is observed in the intra-ply region, unlike the previous unmodified RVE, shown in Fig. 5.9 (a). Hinz et al. (2009) showed experimentally that this intense shear deformation near the ply boundary eventually led to the development of distorted cracks/voids and in some cases debonding around isolated fibres located within the region.
For an interfacial strength of $\tau_{int} = 60$ MPa, the matrix rich RVE shows very similar results to that of the unmodified RVE with the same fibre-matrix interface parameters. Again, the ML case shows a slightly higher shear strength than the TML case, as shown in Fig. 5.10, which is attributed to the increased ISS acting at fibre-matrix interfaces, as already discussed. The progression of damage through the matrix rich RVE is similar to before, with debonding initiating at closely neighbouring fibres aligned to the main tensile loading axis of the RVE. Figures 5.12 (a) and (b) show that an interface dominated fracture path forms for both the ML and TML cases, respectively. Also, it is worth noting that the observed fracture patterns for the ML case and TML case are different, highlighting the effect of thermal residual stress on the microscopic stress state and, consequently, to the onset and evolution of local damage processes. Thus, for a weak fibre-matrix interface, damage tends to be concentrated in
the intra-ply region as interfacial cracks can easily propagate. Whereas, for a strong fibre-matrix interface, damage in the intra-ply region is limited, due to the reinforcing effect of the surrounding fibres, but instead is concentrated near the ply boundary.

![Figure 5.12: Final fracture path of the modified ‘matrix rich’ RVE for an interfacial strength of 60 MPa for the (a) ML case and (b) TML case (Note: a deformation scale factor of 2 has been used in the above images).](image)

**Effect of Interface Fracture Energy**

The influence of interfacial fracture energy on the transverse shear behaviour was examined by considering behaviour of the already studied fracture energy of $\Gamma=10$ J/m² and three further fracture energies, i.e., $\Gamma=2.5$ J/m², $\Gamma=25$ J/m² and $\Gamma=100$ J/m². Figure 5.13 shows the transverse shear response of an RVE which had an interfacial strength of $t_\text{int}^{\text{fr}}=60$ MPa for the range of interfacial fracture energies considered. The effects of increasing the fracture energy are similar to those outlined for the transverse tensile case, discussed in Chapter 4, with beneficial effects being seen in the transverse shear strength and also the strain to failure of the material. Increasing the fracture energy reduces the rate of softening and, consequently, the ultimate displacement at failure (as shown by $\delta_m^{\text{fr}}$ in the traction separation law in Fig. 4.3) of the fibre-matrix interface. This not only affects the behaviour at the fibre-matrix interface, but can have a significant effect on the interaction of other microscopic damage mechanisms in adjacent regions of the microstructure.
yielding in the intermediate matrix ligaments, as shown in Fig. 5.14 (b). The slow rate shown in Fig. 5.14 (c). Although extensive damage had occurred over the entire RVE, increased transverse shear strength and a larger strain to failure of the material, as mechanism, attenuating the stress concentration.

Interestingly, this RVE underwent the greatest amount of damage prior to failure. As interfaces and the small matrix bridges which formed between neighbouring debonded interfaces, the transverse shear strength was obtained for the lowest (Γ=2.5 J/m²) and highest (Γ=100 J/m²) fracture energies considered, as shown in Figs. 5.14 (a) and (b), respectively. For a low fracture energy (Γ=2.5 J/m²), damage initiated in the form of a small number of concentrated interface cracks between closely neighbouring fibres. These cracks quickly propagated across the RVE to neighbouring interfaces to form a fracture path, which was perpendicular to the main principal tensile loading axis, as shown in Fig. 5.14 (a). Due to the high rate of softening of cohesive zones, the transverse shear strength was reduced, as shown in Fig. 5.14 (c), and damage was limited to the fibre-matrix interfaces and the small matrix bridges which formed between neighbouring debonded interfaces. Meanwhile, the highest transverse shear strength was obtained for the highest fracture energy considered (Γ=100 J/m²), as shown in Fig. 5.14 (c), and, interestingly, this RVE underwent the greatest amount of damage prior to failure. As shown in Fig. 5.14 (b), fibre-matrix debonding was widespread across the RVE and the slow rate of softening at the interface promoted extensive yielding in matrix regions adjoining interfacial cracks. This plastic softening subsequently acted as a toughening mechanism, attenuating the stress concentrations at interface crack tips resulting in increased transverse shear strength and a larger strain to failure of the material, as shown in Fig. 5.14 (c). Although extensive damage had occurred over the entire RVE, final fracture was a result of coalescence of a number of interfacial cracks through yielding in the intermediate matrix ligaments, as shown in Fig. 5.14 (b). The slow rate
of softening leads to a higher transverse shear strength and means that damage is more effectively dissipated over the entire RVE, producing favourable response characteristics, such as increased strength and higher strain to failure.

Figure 5.14: Progression of damage through an RVE with different fracture energies: (a) \( \Gamma = 2.5 \text{ J/m}^2 \) (b) \( \Gamma = 100 \text{ J/m}^2 \) and (c) stress-strain response for different fracture energies (Note: a deformation scale factor of 2 has been used in the above images).
5.3.3 Effect of Thermal Residual Stress on Failure Surface

Finally, failure of the material was also predicted under a combination of transverse shear and transverse normal loads to examine the effect of thermal residual stress on the failure surface in the transverse plane. For the combined loading case, in addition to the total shear displacement (δs) applied to the RVE, a horizontal normal displacement (δn) was also applied to the RVE at the active control node n2, as shown in Fig. 5.15. By varying the ratio of the applied transverse shear/normal displacements (δs/δn), a failure envelope for the material was constructed for both the ML and TML cases. For the TML case, the thermal load was applied in a similar manner to that described in Section 5.2.1.

![Figure 5.15: Combined transverse normal and shear displacements applied to an RVE.](Image)

Figure 5.16 shows the failure envelope generated for both the ML and TML cases in the σ22 − τ23 stress space, where an interface strength of t_n/s = 60 MPa and a fracture energy of Γ = 10 J/m² was assumed, meaning that failure was dominated by interface cracking. It is noticeable that the two failure surfaces are largely similar, however, as was found by Zhao et al. (2006), the inclusion of thermal residual stress has meant the TML case has been shifted and slightly contracted compared to the ML case. This shift in the fracture surface occurs as, for tension dominated loading, thermal residual stress has a beneficial effect on the failure strength. This is due to the large compressive stresses which exist at the interface following thermal cool-down from cure temperature, which effectively delay the onset of debonding, as discussed in Chapter 4. As the loading begins to become shear dominated, the presence of thermal
residual stress begins to affect the fracture surface negatively, as increased interfacial shear stress following the thermal loading phase contributes to earlier failure of the material, as outlined in Section 5.3.1. For compression dominated loading, thermal residual stress shows slightly negative effects as failure at the interface must occur due to shear failure (note: a compressive stress at the interface cannot cause debonding to occur). The largest difference between the ML and TML failure surfaces occurs for a loading ratio of, $\delta_y/\delta_n = -4$. Interestingly, the fracture path for this loading ratio comprises of a series of interfacial cracks orientated parallel to the horizontal shear loading axis, as shown in Fig. 5.16 (c), indicating failure at these interfaces was shear dominated. As shown in Figs. 5.16 (a)-(d), the orientation of the final fracture path varied as a function of the ratio of the applied transverse shear and normal displacements. Interestingly, the orientation of the failure plane observed in the micromechanical model under transverse compression (i.e. $\delta_n = -1$), shown in Fig. 5.16 (d), is inclined at 54° to the 3-axis, giving very good agreement with experimental observations which, for fibre reinforced epoxy systems, are usually in the region of 50-56° with respect to the plane perpendicular to the loading axis (González & Llorca 2007a) (for further validation of the micromechanical model, experimental transverse compressive could be carried out on the HTA/6376 laminate to determine the exact orientation of the failure plane). The effects of thermal residual stress on the fracture surface predicted here are similar to those in Zhao et al. (2006), however they are much less pronounced. Due to the brittle nature of the damage model used by Zhao et al. (2006), a large difference is seen between the ML and TML fracture surfaces. However, it has been shown here that constituent non-linear behaviour, due to matrix yielding and the softening process at the interface, relieves the effects of thermal residual stress during the fracture process which results in similar failure surfaces for the ML and TML cases.
Figure 5.16: Failure surface generated by micromechanical models using combined transverse normal and shear loading regime.

Following the recent work carried out in the World Wide Failure Exercise (WWFE) (Hinton et al. 2004), a number of failure theories have been compared to experimental predictions of lamina failure. However, material failure in the transverse normal and shear planes is notoriously difficult to predict experimentally due to the complex nature of the stress state. Thus, micromechanics provides the clear advantage that it can be used to evaluate the performance of ply-level failure criteria for complex stress states, such as those analysed here, without the need for experimental testing. One of the most widely used for failure predictions of composite lamina was proposed by Hashin (1980), whose criteria is based on the assumption of a quadratic interaction of the normal ($\sigma_{22}$) and shear ($\tau_{23}$) stresses acting, such that in the case of tensile normal stresses,

$$
\frac{\sigma_{22}}{S_{22}^T} + \left(\frac{\tau_{23}}{S_{23}}\right)^2 = 1
$$

while in the presence of compressive normal stresses the following criteria was proposed,

$$
\left[\frac{S_{22}^C}{2S_{22}}\right]^{-1} \frac{\sigma_{22}}{S_{22}^C} + \left[\frac{S_{22}^C}{2S_{23}}\right]^2 + \left[\frac{\tau_{23}}{S_{23}}\right]^2 = 1
$$
where $S_{22}^c$ and $S_{22}^t$ are the transverse compressive and tensile strengths of the lamina, respectively, while $S_{23}$ is the transverse shear strength of the lamina. Shown in Fig. 5.16 is the prediction of the failure surface using the Hashin criteria in the transverse stress space (i.e. Eqs. 5.1 and 5.2). For the analysis carried out, the values for $S_{22}^c$, $S_{22}^t$ and $S_{23}$ are based on the micromechanical model’s prediction of transverse compressive, tensile and shear strengths, respectively, for the ML case. The values obtained are given in Table 5.2.

Table 5.2: Strength values predicted by micromechanical model.

<table>
<thead>
<tr>
<th>$S_{22}^c$</th>
<th>$S_{22}^t$</th>
<th>$S_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>166.2</td>
<td>66</td>
<td>55.75</td>
</tr>
</tbody>
</table>

The comparison of the failure surfaces in Fig. 5.16 shows that the quadratic interaction of normal and shear stresses, proposed by Hashin (Eqs. 5.1 and 5.2), provides an adequate prediction of material failure under these combined stress states. For transverse shear and compressive loading ($\sigma_{22} < 0$), the Hashin prediction (Eq. 5.2) is almost superimposed with the predictions of the micromechanical simulations. Meanwhile, for transverse shear and tensile loading ($\sigma_{22} > 0$), Hashin’s prediction (Eq. 5.1) is accurate for tension dominated loading and only slightly overestimates failure for high values of $\delta_s/\delta_n$. Thus, it has shown through micromechanics that the simple assumption made by Hashin, i.e. that failure is governed by a quadratic interaction of normal and shear stresses, is adequate to predict failure in this stress space. It should be noted however that the accuracy of Hashin’s predictions of failure in the transverse plane is dependant upon suitable determination of $S_{23}$, which can be difficult to measure experimentally. Also, one of the drawbacks of Hashin’s model is that it does not predict the plane of failure, whereas the micromechanical simulations are shown to explicitly predict the orientation of the failure plane for each loading ratio. This is shown by the unique fracture paths exhibited by each of the RVE inserts in Fig. 5.16 (a) – (d). Furthermore, it has been shown in Chapters 4 and 5 that, for transverse tensile and shear loading, significant non-linear behaviour is observed before the peak stress is reached. This is true for the combined loading regimes analysed here and, while Hashin provides an adequate description of the ultimate failure of the ply, it fails to predict the development of sub-critical damage mechanisms, which contribute to overall laminate degradation, as outlined in Chapter 2.
5.4 Concluding Remarks

A micromechanical model was used to examine the influence of the intra-ply properties on the transverse shear deformation of a carbon fibre/epoxy composite material. It was shown that thermal residual stress had a significant effect on the interfacial stress state and its presence was enough to alter the initial location of damage and indeed the final fracture path through the RVE. Its overall influence on the macroscopic response was not as pronounced, particularly when shear deformation is dominated by the matrix phase, although a slight reduction in transverse shear strength was seen when failure was governed by interface fracture. Under combined transverse normal and shear loading, it was found the transverse fracture surface was slightly contracted by the presence of thermal residual stress.

The most desirable transverse shear response was obtained when the matrix underwent significant yielding, which occurred for either a strong fibre-matrix interface or for a fibre-matrix interface with a high fracture energy. It was found that for a higher interfacial fracture energy, damage dissipated over the entire microstructure, through a combination of matrix yielding and gradual fibre-matrix debonding, resulting in increased transverse shear strength and a higher strain to failure. Meanwhile, for a strong fibre-matrix interface (i.e. $t_{u/s}^{m} > c$), damage in the intra-ply region was found to be limited, due to the reinforcing effect of the surrounding fibres. Instead, it was found that the region near the ply boundary was more susceptible to yielding behaviour, due to the locally low fibre volume fraction in that region. Whereas, for a weak fibre-matrix interface (i.e. $t_{u/s}^{m} < c$), damage tended to be concentrated in the intra-ply region, as interfacial cracks could easily propagate between closely neighbouring fibres. It should be remembered that the analysis was carried out assuming that the parameters defining behaviour at the fibre-matrix interface were the same for Mode I and Mode II type failures. The mixed-mode behaviour of interface crack growth for different Mode I and Mode II parameters (i.e. strength and fracture energy) warrants further investigation. The model developed herein also showed similar intra-ply damage characteristics as those observed using in-situ SEM experiments by Hinz et al. (2009) and could thus prove useful for determining optimum constituent properties for composite material systems.
Chapter 6

A MATLAB Micromechanics Toolbox for Composite Materials

6.1 Introduction

In this chapter, a Composite Micromechanics Toolbox is developed in MATLAB which provides efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. The findings from Chapters 4 and 5 have shown that the intra-ply properties, such as interfacial properties, local fibre distribution, local fibre volume fraction and thermal residual stress, have a significant effect on the damage and failure behaviour of the material under loading in the transverse plane (Vaughan & McCarthy 2011a, b). As a result of the dependence of the macroscopic properties on microscopic phenomenon, the field of multiscale modelling, or more specifically its implementation using commercial finite element codes, is receiving much attention from academic researchers (Ghosh et al. 2007), aircraft manufacturers (de Boer & Poort 2010) and commercial software developers (Firehole Technologies Inc. 2009) alike. The development of such design tools, which adopt multiscale concepts for the analysis of composite materials, provides a more fundamental approach for predicting structural behaviour, facilitating a more complete understanding of composite failure processes.

The work carried out in this thesis has shown that computational micromechanics can provide detailed predictions of microscale damage and
deformation processes in fibre reinforced composite materials. While access to high performance parallel computing resources allows multi-fibre statistically equivalent RVEs to be solved relatively quickly, the pre- and post-processing stages of micromechanical analyses can remain a complicated time-consuming task. The pre-processing stage can require strict mesh generation criteria and the manipulation of large amounts of data to define suitable nodesets for the correct implementation of periodic boundary conditions. Meanwhile, the post-processing stage can involve the analysis of local stress and strain fields to determine homogenised properties of the material. For an experienced analyst, pre- and post-processing times can obviously be reduced, however, to advance the use of multiscale concepts towards industrial applications, analysis techniques need to be simplified. As a result, the COmposite MicroMechanics (COMM) Toolbox was developed in MATLAB which enables efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. The COMM Toolbox provides a simple, convenient environment for creating, submitting, monitoring, and evaluating results from micromechanical analyses. A number of case studies are carried out which highlight the functionality of the newly developed COMM Toolbox. The findings from these case studies also provide further insight into the behaviour of composite materials under loading in the transverse plane.

This chapter is organised as follows. In Section 6.2, the development of the COMM Toolbox is outlined. In Section 6.3, a number of case studies are presented which highlight the features of the COMM Toolbox. Finally, Section 6.4 summarises the main findings and provides some concluding remarks on the work carried out in this chapter.

6.2 Development of the COMM Toolbox

The COmposite MicroMechanics (COMM) Toolbox was developed in MATLAB and its function is to provide efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. The COMM Toolbox uses ABAQUS as its finite element solver since advanced non-linear and fracture modelling techniques are readily available. The COMM toolbox operates through a series of graphical user interfaces (GUIs) which carry out all tasks involved in micromechanical
analyses. The core tasks include microstructure generation, preparation of input files (either linear or non-linear), job submission and evaluating results (homogenisation). In addition, the COMM Toolbox provides the capability for the statistical analysis of fibre distributions, submission of jobs to parallel computing resources and active job monitoring. This section describes the operation of the main GUIs associated with the COMM Toolbox.

The COMM Toolbox can be initialised through the main MATLAB window by selecting Start → Toolboxes → Micromechanics Analysis → COMM Toolbox, as shown in Fig. 6.1.

Figure 6.1: Initialising the COMM Toolbox through the main MATLAB window.

6.2.1 Main COMM Toolbox GUI

The main GUI of the COMM Toolbox is shown in Fig. 6.2. Its primary function is to generate fibre distributions, through the use of a number of algorithms which have already been discussed in this thesis. It also provides access to further analysis options available in the COMM Toolbox, such as pre- and post-processing of finite element models. The components of the main COMM Toolbox GUI have been identified in Fig. 6.2 and these are described as follows,
This drop-down menu allows the user to select the type of fibre distribution to be generated. Currently, the fibre distributions available in the COMM Toolbox are the Nearest Neighbour Algorithm (NNA) (Vaughan & McCarthy 2010), the Hard-Core Model (HCM) and both Hexagonal and Square Periodic arrays. The NNA, shown in Fig. 6.3 (a), allows high fibre volume fraction, statistically equivalent RVEs to be generated. The widely used Hard-Core Model, shown in Fig. 6.3 (b), allows non-uniform fibre arrangements of up to ~54% fibre volume fraction to be generated. Meanwhile, both Hexagonal and Square Periodic arrays, shown in Fig. 6.3 (c) and (d), respectively, provide simplified fibre arrangements which can be computationally inexpensive, compared to either the NNA or HCM.
The RVE Controls allow the user to define the parameters of the RVE being generated. In the case of the Nearest Neighbour Algorithm, the user must specify the RVE size and, if required, can select the ‘NNA Properties’ push button to initialise the NNA Properties GUI which provides further options regarding the fibre distribution generated by the NNA. The NNA Properties GUI, shown in Fig. 6.4, allows the user to modify the parameters describing the diameter distribution function and the $1^{\text{st}}$ and $2^{\text{nd}}$ nearest neighbour distribution functions, meaning the NNA can adapt to create fibre distributions which have lower or higher fibre volume fractions. Upon execution of the ‘Generate’ push button located on the Main COMM Toolbox GUI, shown in Fig. 6.2, these parameters are used to generate an RVE which is subsequently plotted in the RVE Display window, also shown in Fig. 6.2.

Figure 6.3: Fibre distributions available in the COMM Toolbox: (a) Nearest Neighbour Algorithm (b) Hard-Core Model (c) Hexagonal Periodic Array and (d) Square Periodic Array.
In the case of the Hard-Core Model, the user must specify the RVE size and the desired fibre volume fraction of the RVE. The user may modify the fibre diameter by selecting Edit → HCM Properties from the main menu bar (shown in Fig. 6.2). Like before, upon execution of the ‘Generate’ push button, these parameters are used to generate an RVE microstructure and this is plotted in the RVE Display window.

Meanwhile, for either the Hexagonal or Square Periodic arrays, the user must also specify the fibre volume fraction and upon execution of the ‘Generate’ push button, the user is prompted to enter the length of arrays in both x- and y-directions. The resulting fibre array is plotted in the RVE Display window, as before.

(c) **RVE Display**

As explained above, the RVE generated by the COMM Toolbox is displayed in this window. By selecting File → Save from the main menu bar, the figure in the RVE Display window may be saved as either an Enhanced Meta File (.emf), a Bitmap (.bmp) or a MATLAB Figure file (.fig).

(d) **Statistical Analysis**

The ‘Statistical Analysis’ push button initialises the Statistical Analysis GUI, as shown in Fig. 6.5. The function of the Statistical Analysis GUI is to comprehensively characterise the fibre arrangement in the RVE using a number of statistical functions. The COMM Toolbox determines the 1\textsuperscript{st} and 2\textsuperscript{nd} nearest neighbour distribution functions, the radial distribution function and the second-order intensity function of an RVE and displays these functions in the Statistical Analysis GUI, as shown in Fig. 6.5.
As discussed in Chapter 3, these functions characterise both the short and long range interaction of fibres in the RVE. Using the ‘Export’ push button, shown in Fig. 6.5, the COMM Toolbox exports this data to a Microsoft Excel worksheet, providing an efficient method for the statistical analysis of fibre distributions.

(e) Laminate Properties

The ‘Laminate Properties’ push button initialises the Laminate Properties GUI, shown in Fig. 6.6 (a). The function of the Laminate Properties GUI is to determine effective properties of the RVE stored in the current workspace. In the Analysis Options panel, the user can designate the components of the laminate properties to be determined by selecting the check boxes shown in Fig. 6.6 (a). To determine \( E_{11}, E_{22}, E_{33} \) and \( G_{23} \), the COMM Toolbox carries out a two-dimensional generalised plane strain analysis while to determine \( G_{12} \) and \( G_{13} \) a three-dimensional model is used. By default, the constituent material properties used by the COMM Toolbox are set to those of HTA carbon fibre and 6376 epoxy matrix, which were given in Chapter 3 (Table 3.1). However, the user may modify the constituent material properties by clicking the ‘Material Properties’ push button located on the Laminate Properties GUI, shown in Fig. 6.6 (a). The Material Properties GUI, shown in Fig. 6.6 (b), allows the fibre
Appendix B). The Python script is executed from the MATLAB environment using the finite element model (an example of one of these python scripts is contained in Appendix B). The process requires a suitable mesh to be generated, the application of periodic boundary conditions, submission of input files to the ABAQUS solver and post-processing of data to evaluate results. These tasks are carried out by the COMM Toolbox as automated background processes and are shown schematically in Fig. 6.7, while their implementation is described in detail below.

For the RVE shown in Fig. 6.7 (a), the COMM Toolbox generates a Python script (job-name.py) containing a series of scripting interface commands which create the finite element model (an example of one of these python scripts is contained in Appendix B). The Python script is executed from the MATLAB environment using the command, dos('abaqus cae noGUI=job-name.py'), which initialises the ABAQUS Python interpreter. This is carried out as a background process and the Python scripting interface commands create the RVE geometry, assign fibre/matrix section properties, generate a mesh and write the details to an ABAQUS Input File (job-name.inp), as shown in Figs. 6.7 (b) and (c).

Figure 6.6: (a) Laminate Properties GUI and (b) Material Properties GUI.

Upon the execution of the ‘Submit’ push button, shown in Fig. 6.6 (a), the COMM Toolbox carries out a series of tasks to determine effective properties of the RVE. The process requires a suitable mesh to be generated, the application of periodic boundary conditions, submission of input files to the ABAQUS solver and post-processing of data to evaluate results. The material properties are assumed to be isotropic, again defined in terms of Young’s modulus and Poisson’s ratio. The Material Properties GUI also contains a number of disabled features which are used for defining thermal and non-linear material behaviour, which will be discussed in Section 6.2.2.
From the ABAQUS Input File (*job-name.inp*), the nodal co-ordinates (stored under the *Node* heading) are imported to the MATLAB workspace and the COMM Toolbox creates a series of nodesets and constraint equations to prescribe periodic boundary conditions to the RVE, as shown by Fig. 6.7 (d). The COMM Toolbox writes these details to the ABAQUS Input File (*job-name.inp*) and executes it from the MATLAB environment using the command, `dos('abaqus job=job-name.inp')`, which submits the job to the ABAQUS solver. Upon job completion, a further Python script is used to extract results from the ABAQUS output database file (*job-name.odb*), shown in Fig 6.7 (e), and the COMM Toolbox calculates the effective properties, as shown in Fig. 6.7 (f). All tasks shown in Fig. 6.7 are carried out by the COMM Toolbox as background processes and require no further input from the user. Once effective properties have been determined, they are displayed in the listbox on the Laminate Properties GUI, shown in Fig. 6.6 (a).

![Figure 6.7: Tasks carried out by the COMM Toolbox to determine effective properties for an RVE.](image)

(f) **ABAQUS Analysis**

The ‘ABAQUS Analysis’ push button located on the Main COMM Toolbox GUI, shown in Fig. 6.2, initialises the ABAQUS Analysis GUI which allows the user to interface with the ABAQUS solver.
create ABAQUS Input Files for non-linear micromechanical analysis. This feature is described in more detail in Section 6.2.2.

6.2.2 Pre-processing Abaqus Input Files for Non-Linear Analysis

The COMM Toolbox can create non-linear ABAQUS Input Files using the ABAQUS Analysis GUI, shown in Fig. 6.8. The ABAQUS Analysis GUI may be initialised using the ‘ABAQUS Analysis’ push button located on the Main COMM Toolbox GUI, shown in Fig. 6.2. Its function is to allow efficient pre-processing of ABAQUS Input Files for two-dimensional generalised plane strain analysis and provide a convenient job submission system for the ABAQUS solver. The ABAQUS Analysis GUI allows the user define various parameters of a micromechanical model, e.g. material properties, mesh density or boundary conditions, using the ABAQUS Toolbar, as shown in Fig. 6.8. The main components of the ABAQUS Analysis GUI are identified in Fig 6.8 and these are described as follows,

![ABAQUS Analysis GUI](image)

Figure 6.8: ABAQUS Analysis GUI for pre-processing files for non-linear analysis.

(a) Material Properties

The ‘Material Properties’ push button initialises the Material Properties GUI which enables the user define the thermal and mechanical properties of the constituent materials, as shown in Fig. 6.9. The fibre properties may be defined as either isotropic,
in terms of Young’s modulus and Poisson’s ratio, or orthotropic, in terms of the engineering constants. If a thermal analysis is being carried out, values for either isotropic or orthotropic thermal expansion coefficients may be defined. Meanwhile, the matrix properties are assumed to be isotropic and non-linear behaviour may be specified by selecting the Mohr-Coulomb plasticity option. This requires the user to enter the cohesion stress and friction angle of the material, as shown in Fig. 6.9. For all the parameters above, default values are initially displayed which describe the behaviour of HTA carbon fibres and 6376 epoxy matrix.

![Material Properties GUI](image)

**Figure 6.9: Material Properties GUI.**

(b) **Mesh Properties**

The ‘Mesh Properties’ push button initialises the Mesh Properties GUI, shown in Fig. 6.10. The Mesh Properties GUI allows the user to define the global seed size used in mesh generation. It also allows a cohesive section to be included at the fibre-matrix interface to predict the onset and evolution of fibre-matrix debonding. The behaviour of the cohesive section is governed by a standard bi-linear traction separation law, which was outlined in detail in Chapter 4. The user defines the behaviour of the cohesive section in terms of the fibre-matrix interface strength, fracture energy and initial elastic stiffness, as shown in Fig. 6.10. The user may also modify the viscosity coefficient, which is used to aid the convergence of cohesive sections.
Incrementation settings for each analysis step, such as the maximum number of increments and the increment size.

The ‘Loads/Boundary Conditions’ push button initialises the Loads/Boundary Conditions GUI, shown in Fig. 6.11 (a), which enables the user to prescribe a thermal and/or mechanical loading step for the given analysis. For a thermal load, the user may apply a temperature change, $\Delta T$, which is applied globally to each node in the model, as shown in Fig. 6.11 (b). For a mechanical load, the user can prescribe either a transverse normal displacement ($\delta_n$), transverse shear displacement ($\delta_s$) or combined transverse normal/shear displacements, as shown in Fig. 6.11 (b). As outlined in Chapters 4 and 5, these displacements are applied to active control nodes, $n_2$ and $n_4$, as shown in Fig. 6.11 (b). The Load/Boundary Conditions GUI also allows the user to configure the time incrementation settings for each analysis step, such as the maximum number of increments and the increment size.

Figure 6.11: (a) Loads/Boundary Conditions GUI (b) Boundary conditions applied to an RVE.
The ‘Analysis Outputs’ push button initialises the Analysis Outputs GUI, shown in Fig. 6.12. This allows the user to select a number of field or history output requests for the current analysis. By default, the COMM Toolbox outputs stress, strain and displacement components for an analysis, however, the Analysis Outputs GUI enables the user to request supplementary field outputs, such as plastic strain components, cohesive element variables or element temperature values, depending on the type of analysis being carried out. By default, the history output of the reaction forces and spatial displacements at the control nodes is stored and written to the ABAQUS data file (*job-name.dat), as shown in Fig. 6.12. This data is required for a number of post-processing features available in the COMM Toolbox, which are described in more detail in Section 6.2.3.

This listbox displays a preview of the ABAQUS Input File which the COMM Toolbox will create, as shown in Fig. 6.8. The contents are updated each time a model parameter is edited using the ABAQUS Toolbar menu, i.e. upon completion of any of the steps (a)-(d), described above. For example, once the user edits the material properties using the Material Properties GUI, shown in Fig. 6.9, the contents of the ABAQUS Input File are automatically updated to include these parameters under the *Material option in the Input File Preview, as shown in Fig. 6.8. Once the user has defined all the parameters describing the model behaviour the ‘Create’ push button is
clicked and the COMM Toolbox prompts the user to enter a job name and subsequently creates the ABAQUS Input File (*job-name.inp*). The COMM Toolbox follows a similar procedure to that described in Section 6.2.1 (e) to prescribe periodic boundary conditions and create the ABAQUS Input File.

(f) Submission Options

The Submission Options panel allows the selection of any ABAQUS Input File from the current directory using the listbox on the ABAQUS Analysis GUI, shown in Fig. 6.8. The input file can be submitted to run on either the local machine or parallel computing resources. In the case of the Local Machine, the analysis is carried out in the current working directory and the ABAQUS Input File (*job-name.inp*) is submitted, upon execution of the ‘Submit’ push button, to the ABAQUS solver by the COMM Toolbox through the DOS command, `dos('abaqus job=job-name interactive')`.

In the case of Parallel Resources being selected, the job is submitted to run on the AMPS parallel computing cluster located at the University of Limerick. This capability was implemented by remotely connecting the COMM Toolbox to the AMPS parallel computing cluster using an open source Secure Shell (SSH) Toolbox, which was developed for MATLAB by Nehrbass et al. (2006). The SSH Toolbox uses the widely recognised ‘PuTTY’ SSH client to connect between the Windows and Linux based systems. This allows the execution of commands from the COMM Toolbox to the remote host.

Upon execution of the ‘Submit’ push button located on the ABAQUS Analysis GUI, shown in Fig. 6.13, the COMM Toolbox connects to the AMPS cluster, as shown in Fig. 6.13 (a). This requires the user to provide authentication, as shown in Fig. 6.13 (b). Finally, the user then defines the number of nodes and processors the job requires, as shown in Fig. 6.13 (c), and these details are written to a torque (submission) script. The COMM Toolbox then copies the ABAQUS Input File to the AMPS cluster drive and executes the torque script which launches the job on the AMPS queuing system. This submission process can be easily modified for submission to other remote parallel computing resources by changing the Secure Shell (SSH) connection properties, i.e. the SSH host and user names. These may be modified by selecting Edit → SSH Properties on the main menu bar on the ABAQUS Analysis GUI, shown in Fig. 6.13.
Results GUI are identified in Fig. 6.14 and may be described as follows.

- The ABAQUS Results GUI allows the user to access ABAQUS output active jobs.

This push button initialises the ABAQUS Results GUI which enables the user to efficiently post-process results from micromechanical analyses. This feature is discussed in detail in Section 6.2.3.

6.2.3 Post-Processing Abaqus Results

The ‘Results’ push button located on the ABAQUS GUI, shown in Fig. 6.8 initialises the ABAQUS Results GUI, shown in Fig. 6.14. Its function is to efficiently post-process results from micromechanical analyses and also to monitor the progress of active jobs. The ABAQUS Results GUI allows the user access ABAQUS output database files, display and/or extract stress-strain response data from an analysis and view the increment summary of an active job. The main components of the ABAQUS Results GUI are identified in Fig. 6.14 and may be described as follows,

- Output Database Directory
- Results Options
- Stress-Strain Response
- Status File Preview

Figure 6.13: Submitting jobs to parallel computing resources using the COMM Toolbox.

Figure 6.14: GUI for post-processing Abaqus output database files.
(a) **Output Database Directory**

This listbox displays all the ABAQUS output database files (job-name.odb) located in the current directory. Upon execution of the ‘Open’ push button, the COMM Toolbox opens the selected output database file in the ABAQUS/CAE window.

(b) **Results Options**

The Results Options panel allows the user to access results from the selected ABAQUS output database file through either the ‘Plot’ or ‘Export’ options, shown in Fig 6.14 as push buttons. Results are available as stress-strain data determined in either the 2- or 3-direction from the active control nodes, $n_2$ and $n_4$, which were identified in Fig. 6.11 (b). The ‘Plot’ push button displays the stress-strain response from a given node on the adjacent axes (shown in Fig 6.14 (c)), while the ‘Export’ push button automatically exports the selected data to a Microsoft Excel worksheet (job-name.xls). The COMM Toolbox uses the ABAQUS data file (job-name.dat) to access results, which contains the nodal outputs of reaction forces and displacements. As the ABAQUS data file is updated throughout an analysis, this enables the user to obtain a live update of the current stress state in a model.

(c) **Stress-Strain Response**

As explained above, the stress-strain response determined from one of the active control nodes is displayed here.

(d) **Status File Preview**

This listbox enables the user to monitor the progress of active jobs by displaying a preview of the ABAQUS status file (job-name.sta). This file stores the status of increment summaries which are written by ABAQUS during an analysis, revealing the current stage of the analysis.

6.3 **Case Studies using the COMM Toolbox**

To demonstrate the features of the newly developed COMM Toolbox, a number of case studies have been carried out. These case studies further examine the behaviour
of composites under loading in the transverse plane and provide added insight into microscale deformation processes in fibre reinforced composite materials.

6.3.1 Case Study A: Effect of fibre volume fraction on transverse behaviour

To consider the effect of fibre volume fraction ($V_f$) on the transverse behaviour, the COMM Toolbox was used to generate a number of microstructures which had fibre volume fractions of $V_f = 20\%$, $V_f = 40\%$ and $V_f = 59\%$. The NNA was used to generate the microstructures for $V_f = 59\%$, while the Hard-Core Model (HCM) was used to generate microstructures for both $V_f = 20\%$ and $V_f = 40\%$. As discussed in Chapter 2, the HCM has been widely used to generate lower fibre volume fraction microstructures (less than approximately $V_f = 50\%$) for composite materials. It represents the fibres as a set of non-overlapping inclusions which have been randomly distributed within the domain. The MATLAB code (.m file) for the Hard-Core Model is contained in Appendix B. As was carried out for the NNA, developed in Chapter 3, a minimum inhibition distance of 0.1µm between neighbouring fibres was specified in the HCM to allow for adequate discretisation in the inter-fibre region. While this section analyses the effect of fibre volume fraction on the mechanical behaviour of the material, a statistical analysis has also been carried out in order to characterise the fibre distributions which are generated by the NNA (for high fibre volume fraction microstructures) and by the HCM (for low fibre volume fraction microstructures).

Statistical Analysis

To characterise the fibre distributions produced by the NNA and HCM, 20 microstructures were generated using the COMM Toolbox at each fibre volume fraction (i.e. $V_f = 20\%$, $V_f = 40\%$ and $V_f = 59\%$). These measured $165 \times 165 \mu m (\delta=50)$ and a resulting microstructure for each fibre volume fraction is shown in Fig. 6.15. The Statistical Analysis GUI, discussed in Section 6.2.1(d), was used to extract the $1^{st}$ and $2^{nd}$ nearest neighbour distribution functions for these models. Shown respectively in Figs. 6.16 (a) and (b) are the mean values of the $1^{st}$ and $2^{nd}$ nearest neighbour distribution functions for each fibre volume fraction considered. Error bars have been included for each of the functions indicating the maximum and minimum values generated from the models for each data point.
nearest neighbour distribution functions observed here for each fibre volume fraction. For the highest fibre volume fraction, i.e. $V_f = 59\%$, the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distributions exhibit narrow ranges and high peaks occur at distances of 7 $\mu$m and 7.2 $\mu$m, respectively. This is an obvious result of the high fibre volume fraction as there is limited space available for fibres to positions themselves. In contrast, for the lowest fibre volume fraction, i.e. $V_f = 20\%$, the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distribution functions show no observable peak and each distribution exhibits a wide range, highlighting that fibres have no tendency, or indeed obligation, to cluster close to one another. Meanwhile, for $V_f = 40\%$, the characteristics of the nearest neighbour distribution functions are intermediate to those of the highest (i.e. $V_f = 59\%$) and lowest (i.e. $V_f = 20\%$) fibre volume fractions shown. It was shown in Chapter 5 that, under transverse shear loading, the proximity of neighbouring fibres had a significant effect on the interfacial stress state. This suggests that the large difference in the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distribution functions observed here for each fibre volume fraction could affect the failure behaviour under loading in the transverse plane.

Figure 6.15: Fibre distributions generated by the COMM Toolbox for (a) $V_f = 20\%$ (b) $V_f = 40\%$ and (c) $V_f = 59\%$. 

For the highest fibre volume fraction, i.e. $V_f = 59\%$, the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distributions exhibit narrow ranges and high peaks occur at distances of 7 $\mu$m and 7.2 $\mu$m, respectively. This is an obvious result of the high fibre volume fraction as there is limited space available for fibres to positions themselves. In contrast, for the lowest fibre volume fraction, i.e. $V_f = 20\%$, the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distribution functions show no observable peak and each distribution exhibits a wide range, highlighting that fibres have no tendency, or indeed obligation, to cluster close to one another. Meanwhile, for $V_f = 40\%$, the characteristics of the nearest neighbour distribution functions are intermediate to those of the highest (i.e. $V_f = 59\%$) and lowest (i.e. $V_f = 20\%$) fibre volume fractions shown. It was shown in Chapter 5 that, under transverse shear loading, the proximity of neighbouring fibres had a significant effect on the interfacial stress state. This suggests that the large difference in the 1$^{\text{st}}$ and 2$^{\text{nd}}$ nearest neighbour distribution functions observed here for each fibre volume fraction could affect the failure behaviour under loading in the transverse plane.
To examine the effect of fibre volume fraction on the material behaviour, a combined transverse compressive and shear loading regime was used to predict failure envelopes for the material. The COMM Toolbox was used to generate an RVE measuring 66 × 66 µm (δ=20) at each fibre volume fraction under consideration (i.e. \( V_f = 20\% \), \( V_f = 40\% \) and \( V_f = 59\% \)). The behaviour of the constituent materials was assumed to be the same as that used in Chapters 4 and 5. For this combined loading case, a transverse shear load was imposed on the RVEs by applying complimentary

\[ \text{Mechanical Analysis} \]

Figure 6.16: (a) 1\textsuperscript{st} Nearest Neighbour Distribution function and (b) 2\textsuperscript{nd} Nearest Neighbour Distribution function for distributions generated.
horizontal and vertical displacements ($\delta_n/2$) to the active control nodes, $n_4$ and $n_2$, respectively. Meanwhile, the transverse compressive load was imposed by applying a horizontal normal displacement ($\delta_n$) at the active control node $n_2$, as shown in Fig. 6.17. By varying the ratio of the applied transverse shear/normal displacements ($\delta_s/\delta_n$), a failure envelope for each fibre volume fraction was determined in the $\sigma_{22} - \tau_{23}$ stress space.

By varying the ratio of the applied transverse shear/normal displacements ($\delta_s/\delta_n$), a failure envelope for each fibre volume fraction was determined in the $\sigma_{22} - \tau_{23}$ stress space.

Figure 6.17: Boundary conditions applied to an RVE ($V_f = 20\%$) for the combined transverse compressive and shear loading case.

It was shown in Chapter 5 that failure of the material under transverse shear loading could be dominated by fibre-matrix interface failure (for a weak fibre-matrix interface) or by matrix yielding (for a strong fibre-matrix interface). Thus, the analysis carried out here considers both failure modes. For the first case, an interface strength of $t_{ns} = 60$ MPa and a fracture energy of $\Gamma = 10$ J/m$^2$ were assumed, meaning that failure was dominated by fibre-matrix interface failure. Meanwhile, the second case assumes a perfect fibre-matrix interface, meaning that failure was dominated by matrix yielding. Constructing a failure surface for each different case (different fibre volume fractions and fibre-matrix interface strengths) required a large number of models to be generated. The COMM Toolbox allowed for the efficient generation of over 40 different models for this study using the ABAQUS Analysis GUI, described in Section 6.2.2. The ABAQUS Analysis GUI also allowed for convenient job submission to the AMPS
parallel computing cluster. Meanwhile, the Abaqus Results GUI, discussed in Section 6.2.3, was used to extract the stress-strain response of the RVEs at each loading ratio.

Figure 6.18 shows the effect of fibre volume fraction on the transverse failure surface when a fibre-matrix interface strength of $t^o_{n/s} = 60 \text{ MPa}$ and a fracture energy of $\Gamma=10 \text{ J/m}^2$ were assumed. For this interface dominated failure, it was found that reducing the fibre volume fraction actually results in a slight expansion of the transverse failure surface. Figure 6.18 shows only a slight difference between the failure surfaces of 40% and 59% fibre volume fraction, however, the 20% fibre volume fraction shows much higher failure strengths for all loading ratios. This higher strength for lower fibre volume fractions can be attributed to the larger inter-fibre spacing between neighbouring fibres. This was established in Figs. 6.16 (a) and (b) where, for lower fibre volume fractions, the 1st and 2nd nearest neighbour distribution functions showed no observable peak and exhibited a wide range. It was also shown in Section 5.3.1, for the transverse shear loading case, that a larger inter-fibre spacing causes a reduction in the interfacial normal and shear stresses. Thus, in lower fibre volume fraction arrangements, the larger inter-fibre spacing effectively delays the onset of debonding, resulting in higher strengths for each loading ratio. It should also be noted that due to the larger inter-fibre spacing, the propagation of interface cracks to adjacent fibres (due to stress redistribution) is inhibited and promotes further yielding in intermediate matrix regions, leading to higher predicted strengths. In other terms, it is easier for an interface crack to propagate to a neighbouring interface which is closer to it, than to one which is further away. This can be seen when the final plots from the $V_f = 20\%$ case and $V_f = 59\%$ case are compared for a loading ratio of $\delta_t / \delta_s = -2$, as shown in Figs. 6.19 (a) and (b), respectively. While the lower fibre volume fraction RVE ($V_f = 20\%$) results in a higher predicted strength under loading in the transverse plane, it must be remembered that it would be only $\sim 35\%$ as strong as the high fibre volume fraction RVE ($V_f = 59\%$) when loaded in the fibre direction.
Figure 6.18: Effect of fibre volume fraction on transverse failure surface for interface dominated failure.

Figure 6.19: Final deformation for a loading ratio of $\delta_2 / \delta_n = -2$ in RVEs where (a) $V_f = 20\%$ and (b) $V_f = 59\%$.

Figure 6.20 shows the effect of fibre volume fraction on the transverse failure surface for an assumed perfect fibre-matrix interface, such that failure was matrix dominated. In contrast to interface dominated failure (shown in Figs. 6.18 and 6.19), it was found that reducing the fibre volume fraction for matrix dominated failure results in a contraction of the transverse failure surface, as shown in Fig. 6.20. This is caused by the lack of reinforcement in low fibre volume fraction configurations, which allows matrix yield paths to propagate more easily. This can be seen in Figs. 6.21 (a) and (b) which show the deformation in an RVE subject to a loading ratio of $\delta_f / \delta_n = -1$ for the $V_f = 20\%$ and $V_f = 59\%$ cases, respectively. For $V_f = 20\%$, a dominant shear band
forms which is unobstructed by fibres, whereas for $V_f = 59\%$ the high fibre volume fraction inhibits the propagation of matrix yielding as many of the yield paths are arrested due to fibres obstructing their path. It is also interesting to note that, while the low fibre volume fraction RVE, shown in Fig. 6.21 (a), shows a dominant yield path and a relatively small amount of yielding in the rest of the microstructure, the high fibre volume fraction RVE, shown in Fig. 6.21 (b), shows that intense yielding is widespread throughout the microstructure. As was found by increasing the interfacial fracture energy in Section 5.3.2, the widespread yielding over the microstructure has meant that damage is more effectively dissipated over the entire RVE, leading to a higher predicted strength.

Figure 6.20: Effect of fibre volume fraction on transverse failure surface for matrix dominated failure.

Figure 6.21: Final deformation for a loading ratio of $\delta_0/\delta_b = -1$ in RVEs where (a) $V_f = 20\%$ and (b) $V_f = 59\%$.  

163
6.3.2 Case Study B: Effect of fibre distribution on transverse behaviour

This section examines the effect of fibre distribution and fibre diameter on the behaviour of the material under combined transverse tensile and transverse shear loading. Each of the distributions available in the COMM Toolbox has been considered in this study, i.e. NNA, Hard-Core Model, Square Periodic array and Hexagonal Periodic array. To compare the results between the Hard-Core Model and the Nearest Neighbour Algorithm, a fibre volume fraction of 52% was assumed. As discussed in Chapter 3, the NNA uses nearest neighbour distribution functions to assign inter-fibre distances within an RVE. The COMM Toolbox allows the parameters characterising the nearest neighbour distribution functions to be altered, meaning the NNA can adapt to create RVEs having different fibre volume fractions. Shown in Fig. 6.22 are the 1\textsuperscript{st} and 2\textsuperscript{nd} nearest neighbour distributions which were found to produce an RVE with a fibre volume fraction of 52%. It can be seen that compared to the original distributions (i.e. $V_f = 59\%$), the mean nearest neighbour distance has increased and the each distribution exhibits a wider range. This relaxes the constraints in the NNA, so as to allow more space between fibres and hence results in a lower fibre volume fraction RVE of $V_f = 52\%$, which is shown in Fig. 6.23 (a). The RVE produced by the HCM for $V_f = 52\%$ is shown in Fig. 6.23 (b), while the Square Periodic and Hexagonal Periodic arrays (where $V_f = 52\%$) are shown in Figs. 6.23 (c) and (d), respectively.

![Figure 6.22: 1\textsuperscript{st} and 2\textsuperscript{nd} Nearest Neighbour Distribution (NND) Parameters governing inter-fibre distances for fibre volume fractions of 59\% and 52\% generated by the NNA.](image)
The effect of fibre diameter on material behaviour is also considered in this study by modifying the fibre diameter distribution parameters defined by the NNA. Shown in Fig. 6.24 are the fibre diameter distributions which were used in the present study. The distribution denoted by ‘NNA’ has the same parameters as that measured in Chapter 3, i.e. the same as the experimental diameter distribution. Meanwhile, the distribution denoted by NNA-VD (variable diameter) assumes a standard deviation four times that of the original NNA, resulting in a lower peak and wider range in the fibre diameter distribution, as shown in Fig. 6.24. These fibre diameter distribution parameters were used in conjunction with newly defined nearest neighbour parameters (described above) to generate an RVE with $V_t = 52\%$, as shown in Fig. 6.25.
A combined transverse tensile and transverse shear loading regime was used to determine a failure surface for each fibre distribution. The boundary conditions used were similar to those described in Section 6.3.1, however, a transverse tensile load (not a transverse compressive load) was applied to the active control node $n_2$ (shown in Fig. 6.17). Again, the ratio of the applied transverse shear/normal displacements ($\delta / \delta_n$) was varied to determine a failure envelope for each fibre distribution, where a fibre-matrix interface strength of $t_{ns}^o = 60$ MPa and a fracture energy of $\Gamma = 10$ J/m$^2$ was assumed. Figure 6.26 shows the resulting failure surfaces for each of the fibre distributions under consideration. It was found that the distributions generated by the NNA, the NNA-VD and by the HCM predicted very similar strength values for all
loading ratios. This suggests that a large variance in fibre diameter has little effect on the failure behaviour of the material under loading in the transverse plane. Meanwhile, the strengths predicted by the Periodic Square and Periodic Hexagonal arrays are consistently higher than the NNA, NNA-VD or HCM distributions for all loading ratios, shown in Fig. 6.26 as expanded failure surfaces. This over-prediction of material strength can largely be attributed to the regular inter-fibre spacing in periodic fibre arrays. However, the difference between the failure surfaces predicted is less than would be expected when compared to previous linear elastic studies which have compared the performance of periodic and non-uniform fibre distributions (Hojo et al. 2009, Trias 2006b).

Figure 6.26: Transverse failure surface for each of the fibre distributions under consideration.

To investigate the performance of these periodic fibre arrays further, the response of each distribution under a transverse tensile load is shown in Fig. 6.27. Similar to the findings in Fig. 6.26, the overall response of the RVEs generated by the NNA, NNA-VD and HCM show almost identical characteristics and, as a result, only the response from the NNA is shown. While the transverse strength predicted by the periodic fibre arrays are only ~11% greater than those of the NNA, NNA-VD or HCM models, the periodic models greatly underestimate the initial point of failure. This is evident here as both the Square Periodic and Hexagonal Periodic arrays underestimate the onset of debonding (i.e. the beginning of non-linear behaviour in the response curves), compared to the RVE generated by the NNA, by 43% and 51%, respectively.
This is obviously due to the regular inter-fibre spacing which cannot represent the stress state seen in non-uniform composite microstructures. In addition, both Square and Hexagonal Periodic arrays predict a transverse failure strain almost double that of the NNA model.

Figures 6.28 (a) and (b) show the progression of damage in the Hexagonal Periodic array and Square Periodic array, respectively. In both periodic arrays, damage initiates simultaneously across the microstructure at each of the fibre-matrix interfaces (Load Points 1). These periodic interfacial cracks propagate around each of the fibre edges causing some matrix yielding at each of the crack tips. Finally, a number of the interface cracks tend to dominate and a final fracture path forms due the coalescence of a number of these periodic cracks through intense matrix yielding (Load Points 2). It was found in Chapter 4 that, due to the different fibre arrangements generated by the NNA, each micromechanical model exhibited a unique failure path and some variance in failure strengths. This highlights that damage in the microstructure will vary from one point to another, depending on the local fibre arrangement, thus implying that damage is not a periodic process. Although the periodic models showed a comparable transverse strength to the RVE generated by the NNA, both the Hexagonal and Square Array greatly over-estimate the onset of damage and the ultimate strain to failure, clearly highlighting the assumptions of the periodic model and its inability to be used in damage and failure based simulations.
Figure 6.27: Effect of fibre distribution on the transverse tensile response of the material.

Figure 6.28: Progression of fibre-matrix debonding and matrix yielding due to transverse tensile loading the (a) Hexagonal Periodic array and (b) Square Periodic array.
Finally, the progression of damage in the RVE with a variable fibre diameter was similar to that described in Chapter 4. The fibre size appeared to have no effect on the development of fibre-matrix debonding, and interface cracks tended to develop between closely neighbouring fibres which were aligned to the loading direction, irrespective of their size, as shown in Fig. 6.29 (Load Point 1). As the load increases, bands of interfacial cracks develop perpendicular to the loading direction. Within these bands of interfacial cracks, the intermediate matrix regions undergo yielding which allows the coalescence of neighbouring interfacial cracks. Finally, a band of interfacial cracks dominate to form the final fracture path across the RVE, which is perpendicular to the loading direction, as shown in Fig. 6.29 (Load Point 2). These results suggest that the production controls monitoring fibre diameter during the manufacturing process could be relaxed, assuming that the strength in the fibre direction would not be affected.

![Progression of damage in an RVE with a variable fibre diameter.](image)

**Figure 6.29:** Progression of damage in an RVE with a variable fibre diameter.

### 6.4 Concluding Remarks

This chapter has outlined the development of the Composite Micromechanics (COMM) Toolbox which provides efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. As computational power continues to increase, more detailed and advanced multiscale modelling strategies have emerged, which better predict internal damage mechanisms and their effect on structural behaviour. However, the inherent complexity associated with such modelling strategies forms a barrier with respect to their advancement from academic interests to practical industry based implementation. The COMM Toolbox addresses this issue as it provides
a simple, convenient environment for creating complex micromechanical damage models, which facilitate a better understanding of how local deformation mechanisms influence material behaviour at higher length scales.

The COMM Toolbox automates all manual tasks associated with micromechanical analysis of composite materials. These include, microstructure generation, statistical analysis of fibre distributions, preparation of input files (either linear or non-linear), job submission to parallel computing resources, active job monitoring and homogenisation calculations. To demonstrate the functionality of the COMM Toolbox, a number of parametric case studies were carried out which analysed the effect of parameters such as fibre volume fraction, interface strength and fibre distribution on material behaviour, under loading in the transverse plane. It was found that a reduced fibre volume fraction led to an increased predicted strength when failure was dominated by interface cracking. In contrast, it was found that a reduced fibre volume fraction led to a reduction in predicted strength when failure was dominated by matrix yielding. Meanwhile, it was found that periodic fibre arrays did not exhibit the same behaviour, in terms of damage evolution and strength predictions, as non-uniform fibre RVE models and so, it is thus concluded that periodic models are not suitable for damage/failure based predictions.

The COMM Toolbox provides a simple, efficient predictive modelling capability for composite materials, based on the physical interactions of the constituent phases which could guide material system selection or processing conditions. The intellectual overhead in learning to use the COMM Toolbox is low and could be suited to analysts with varying levels of expertise. Importantly, the COMM Toolbox allows the analyst to apply advanced non-linear and fracture modelling techniques without requiring extensive background knowledge. In particular, the COMM Toolbox could prove useful in industrial applications for determining application specific properties for composite material systems by numerically carrying out various parameter studies on variables such as cure temperature and/or interface strength, for example.
Chapter 7

Conclusions and Recommendations for Future Work

7.1 Introduction

This thesis has outlined the development of a micromechanics damage model which has examined the failure behaviour of a carbon fibre/epoxy composite under a range of loading scenarios in the transverse plane. This final chapter summarises the main findings from this investigation and provides concluding remarks with regard to their broader implications. This chapter also makes a number of important recommendations towards the future directions of this work.

7.2 Concluding Remarks

7.2.1 Nearest Neighbour Algorithm

The Nearest Neighbour Algorithm (NNA) was developed and its function was to generate statistically equivalent fibre distributions for high strength composite laminates. Despite the significant influence that manufacturing and processing conditions can have on the fibre distribution in a composite microstructure (Pyrz 1994b, Trias 2005), the majority of recent micromechanical investigations have favoured the use of purely numerical algorithms to generate non-uniform fibre distributions (Romanowicz 2010, Wang et al. 2011). The NNA provides a useful alternative to
purely numerical based models and also to the direct microstructure reproduction approach.

The combined experimental-numerical approach employed by the NNA uses experimentally measured nearest neighbour distribution functions to define the inter-fibre distances and an experimentally measured diameter distribution function to assign fibre diameters in the RVE. This allows the short range interaction of fibres in the microstructure to be reproduced, enabling an accurate representation of the local microscopic stress state. The method was verified against a number of mechanical and statistical criteria to ensure its suitability for subsequent micromechanics damage simulations. The NNA does not require further heuristic steps, such as those seen in fibre stirring/shaking algorithms (Wongsto et al. 2005, Melro et al. 2008), in order to achieve high volume fraction microstructures. Moreover, the distributions generated are geometrically periodic meaning that the NNA does not encounter difficulties associated with experimental reproduction approaches, such as the application of suitable periodic boundary conditions.

The NNA is simple, robust, highly efficient and was shown to reproduce actual fibre distributions for high strength laminated composite materials. One of the unique characteristics of the NNA, compared to most of its counterparts (Wongsto et al. 2005, Melro et al. 2008), is that the fibre volume fraction being produced is not predefined. It is controlled by the experimental functions used as the input parameters, i.e. the nearest neighbour distributions and the diameter distribution of the fibres. It was shown that by changing these input parameters, the NNA could adapt to create a lower fibre volume fraction microstructures, which had a large variance in fibre diameter. This implies that the methodology could easily be applied to other types of composite materials by characterising relevant experimental distributions. The versatile nature of the NNA also means that natural occurring composites, such as bone, which generally exhibit high fibre volume fractions and large variances in fibre diameter, could potentially be modelled.

7.2.2 Micromechanical Behaviour under Loading in the Transverse Plane

The micromechanical model developed herein was used to examine the influence of the intra-ply properties, such as interface strength, interface toughness,
fibre volume fraction, local fibre distribution and the presence of thermal residual stresses, on the failure behaviour of the carbon fibre/epoxy composite, under loading in the transverse plane. The computational framework used to model deformation in the carbon fibre/epoxy composite was similar to that pioneered by Llorca, González and co-workers (González & Llorca 2007, Totry et al. 2008a) where, a cohesive zone model was used to predict the onset of fibre-matrix debonding, while the non-linear behaviour in the matrix phase was modelled using the Mohr-Coulomb plasticity theory. The NNA enabled high fibre volume fraction, statistically equivalent RVEs to be used for the analysis which allowed for meaningful predictions of failure in high strength composite materials, under a range of thermal and mechanical loading scenarios.

It was found that the presence of thermal residual stress, caused by the cooling of the material from cure temperature, altered the microscopic stress state of the composite material significantly. It caused compressive and shear stresses to develop at the fibre-matrix interface, whose magnitude depended upon the proximity of neighbouring fibres. For a sufficiently weak fibre-matrix interface, it was found that thermally induced stresses had a detrimental effect, causing interfacial cracks to develop during the cooling phase. By examining the effect of thermal residual stress on the transverse fracture surface, it was shown that, for tension dominated loading, thermal residual stress was effective in offsetting interfacial decohesion as a result of thermally induced compressive stresses acting at the fibre-matrix interface. These stresses compensated for subsequent tensile stresses developed under transverse tensile loading. Similar results, reporting beneficial effects of thermal residual stress for transverse tensile loading, were also found by Maligno et al. (2008) and Hojo et al. (2009). Meanwhile, for transverse shear or compression dominated loading, it was shown that thermal residual stress had slightly negative effects on the predicted strengths, as a result of interfacial shear stresses which developed during the cooling phase. Interestingly, it was shown that the effect of thermal residual stress on the microscopic stress state was sufficient enough to alter the initial location of damage and indeed the final fracture paths through many of the RVEs analysed.

It is well established that properties of the fibre-matrix interface are crucial to the failure behaviour of fibre reinforced composites (Gamstedt & Sjögren 1999). The findings here have also shown this as well as providing added insight into its role and,
more importantly, the consequences of tailoring/improving its properties on the overall behaviour. It was found that the most desirable material response was obtained when the fibre-matrix interface exhibited a high strength or fracture energy. Any increase to the fibre-matrix interface strength provided a general increase in the transverse tensile and transverse shear strengths. However, it has been shown previously that very high interfacial strengths can lead to low fracture toughness values (Khanna & Shukla 1993, 1994).

Meanwhile, it was found that, under transverse shear loading, increasing the interfacial fracture energy caused widespread matrix yielding, which led to higher macroscopic strength values. This concept seems counter intuitive, however, promoting the occurrence of certain sub-critical damage mechanisms allows the dissipation of energy over the entire material microstructure, resulting in a more favourable response. Importantly, under transverse tensile loading, higher fracture energies inhibited the development of transverse cracks and led to an increase in transverse failure strain of the material under investigation. This has important implications as it is the low strain to failure of transverse plies which causes damage to initiate in cross-ply laminates (Gamstedt & Sjögren 1999). Interestingly, many of the recent research efforts into fibre surface treatments are concerned with introducing a softer, more ductile interface in order to improve the strain to failure of transverse plies (Benzarti et al. 2001). The findings here substantiate many of these research efforts by highlighting that a more ductile fibre-matrix interface will produce a more favourable response under both transverse tensile and shear loading.

Due to the number of competing damage mechanisms involved in the failure process, both the local fibre distribution and local fibre volume fraction can have a significant affect on the onset and evolution of microscopic damage. It was shown that the formation of local damage mechanisms depended on the proximity of neighbouring fibres and their orientation relative to the loading direction. In general, for both transverse tensile and transverse shear loading, it was found that fibre-matrix debonding occurred between closely neighbouring fibres, which were aligned with the direction of the maximum principal stress. In low fibre volume fraction configurations, it was found that matrix yielding could occur more easily, due to the lack of reinforcement provided by the fibres and the ease at which yield paths could propagate into matrix rich regions.
For the transverse shear loading case, this meant that yielding would tend to concentrate near the ply-boundary, where the fibre volume fraction tended to be lower (locally) than the intra-ply region. In high fibre volume fraction configurations, it was found that fibre-matrix debonding could easily propagate. This was attributed to the nearest neighbour distances, which were inevitably closer in high volume fraction configurations.

From a practical viewpoint, the findings from this micromechanical investigation highlight the influence of the manufacturing conditions on the overall failure behaviour. The curing process is crucial in developing suitable adhesion between the fibre and matrix phases. In addition, the cure temperature affects the magnitude of thermal residual stresses, while the cure pressure can affect the fibre distribution in the microstructure (Pyrz 1994b). Importantly, the micromechanical model developed herein was found to produce similar failure patterns to those observed experimentally for similar composite material systems for both thermal (Gentz et al. 2004) and mechanical (Hobbiebrunken et al. 2006, Hinz et al. 2009) loading. Under cyclic loading, the micromechanical model provided novel insight into the microscopic damage accumulation that forms prior to ultimate failure, and clearly highlighted the different roles that fibre-matrix debonding and matrix plasticity play in forming the macroscopic response of the composite. For the loading cycle examined (tension-compression-tension), the micromechanical model predicted non-linear behaviour as a result of fibre-matrix debonding and yielding in the matrix under tensile loading. Upon unloading to zero stress, the model predicted a loss in material stiffness (due to fibre-matrix debonding) and permanent plastic strain (due to matrix yielding) in the material. Upon subsequent compressive loading, the micromechanical model predicted crack closure and load take up between newly formed crack faces. Finally, the micromechanical model showed that the ultimate tensile strength was affected by the accumulation of microscale damage from previous loading cycles. Such detailed predictions of microscale deformation could guide the development of more accurate continuum damage models, which often smear these effects using non-physical material parameters (O’Higgins 2011a, b).
Conclusions and Recommendations

7.2.3 Composite Micromechanics Toolbox

The Composites Micromechanics (COMM) Toolbox was developed to provide efficient pre- and post-processing capabilities for micromechanical analyses of composite materials. High-strength fibre reinforced composites have not been as widely used within industry as their structural performance would suggest. A great deal of this can be attributed to the high cost and complexity associated with their processing techniques, coupled with the intense testing and certification procedures applied to composite structures. The emergence of advanced multiscale predictive capabilities potentially provides material and structural designers with enhanced knowledge and understanding of how composite material systems behave, which could help to reduce time between research phases and the marketplace. However, such modelling techniques require high-levels of expertise and remain, for the most part, academic pursuits. Consequently, the COMM Toolbox was developed to provide greater accessibility to state-of-the-art multiscale/multilevel predictive capabilities and to advance these strategies towards practical industry based implementation.

The COMM Toolbox has automated all manual tasks associated with micromechanical analyses of composite materials, providing a simple, convenient environment for creating, submitting, monitoring, and evaluating results from micromechanical analyses. The COMM Toolbox enables a variety of fibre distributions to be generated, allowing the analysis of either non-uniform or regular fibre arrangements for both low and high fibre volume fractions. The interactive pre-processing capability allows ABAQUS Input Files to be created, which can examine a wide range of thermal and/or mechanical loading scenarios effectively. The COMM Toolbox provides a convenient job submission system to the ABAQUS solver using high performance parallel computing resources and also allows active job monitoring. Finally, the COMM Toolbox enables the efficient post-processing of ABAQUS Output Database files, where important data can be exported to Microsoft Excel for further analysis. The functionality of the above features have been demonstrated through a number of case studies undertaken.

Importantly, the COMM Toolbox means that advanced multiscale modelling concepts, which determine material behaviour based on the physical interactions of the constituent phases, are likely to gain more widespread exposure from potential
academic or industry based interests. In particular, it is thought that COMM Toolbox could prove useful for guiding material system selection or processing conditions in industrial applications, be they aerospace or otherwise. Already, the Nearest Neighbour Algorithm (Vaughan & McCarthy 2010) has generated interest from a number of research institutes, with a number of approaches having been made requesting its use. It is envisaged that the COMM Toolbox could generate similar interest and therefore has the potential to become licensed software.

7.3 Recommendations for Future Work

7.3.1 Micromechanical Modelling

While the work carried out in this thesis has examined the behaviour of composites under loading in the transverse plane in great detail, it is proposed that the model be extended to a three-dimensional RVE, in order to predict all components of stress. This would allow for the application of in-plane, longitudinal and a variety of combined loading scenarios, enabling the prediction of multiple material failure surfaces in three-dimensions.

Further improvement to the micromechanical model would be to account for damage in the matrix. Currently, the model uses a Mohr-Coulomb plasticity law to predict the onset of yielding in the matrix and while this gives a good prediction of yielding behaviour under shear and compression dominated loading, it fails to predict the development of brittle micro-cracks under transverse tensile loading. Recently however, Melro et al. (2009) proposed an elastic-plastic damage model to predict the complicated failure behaviour of epoxy matrices. This model uses Raghava’s criteria (Raghava et al. 1973) (discussed in Chapter 2) to account for the pressure-dependant yielding behaviour of epoxies, while the damage law is based on the parabolic shaped criterion proposed by Fiedler et al. (2005b) (also discussed in Chapter 2). This model also mitigates any damage localisation effects through the use of Bazant’s crack band model (Bazant & Cedolin 1979), thus showing high-potential to overcome the inherent difficulties associated with predicting failure behaviour of epoxies.

Another issue which is receiving much attention from both academia and industry is the accurate prediction of delamination in laminated structures. Premature
Conclusions and Recommendations

failure by delamination has significantly limited the potential strength and toughness of composite structures. Many current state-of-the-art continuum models used to predict delamination assume that it is an independent mechanism to local damage occurring in the intra-ply region (Liu et al. 2011). As already discussed in this thesis, inter-ply delamination can actually occur as a result of intra-ply damage, meaning both inter- and intra-ply cracking are inextricably linked (Gamstedt & Sjögren 1999). To date, few micromechanical studies have been carried out examining this phenomenon, thus, it is proposed that the micromechanical model be extended to examine microscopic damage as it propagates from the intra-ply region to the ply boundary. This would require a three-dimensional model which could assume the existence of 2 plies orientated at $\pm \theta$ to one another, such as that shown for a $0^\circ/90^\circ$ lay-up in Fig. 7.1. Various lay-ups and ply orientations could provide added insight into the delamination process and allow for its accurate prediction in laminated structures.

![Multi-Ply RVE](image)

**Figure 7.1:** Multi-Ply RVE to analyse progression of intra-ply damage to the inter-ply region.

Due to their high specific stiffness and strength, composite materials are employed in a range of structural applications under various environmental conditions, finding increasing uses in both low (Kim et al. 2007) and high (Qi et al. 2001) temperature applications. To date, micromechanical investigations examining the effect of temperature on material behaviour have only considered periodic fibre unit cells and
have assumed linear elastic behaviour of the constituents (Fiedler et al. 2005a). The micromechanical model developed herein has already provided novel insight into the formation of microscale damage during the thermal cool-down from cure temperature and has also examined, in detail, the effect of thermal residual stresses on the transverse behaviour. It is thus proposed that the micromechanical model be used to examine damage and failure behaviour over a range of temperatures, which could represent typical in-service conditions of composite material systems. This study would initially require material characterisation using an environmental test chamber to determine the effect of temperature on the mechanical properties of both the carbon fibre/epoxy composite and neat epoxy resin specimens (the strength of epoxy resins has been shown to be highly dependant on temperature (Fiedler et al. 2005a)). One possible application for this type of study is the use of carbon fibre/epoxy pressure vessels for the storage of cryogenic liquid fuels in aerospace applications (Kim et al. 2007).

While the work carried out in this thesis has focussed on microscale deformation, the ultimate goal in the field of multiscale modelling is to predict structural behaviour of heterogeneous materials based on the physical interactions of their constituents. It is proposed that the micromechanical model developed be used to investigate the feasibility of coupled multi-level simulations for composite materials. Smit et al. (1998) proposed a micro-macro approach to structural analysis which involves a macro-level mesh which has a micro-level RVE assigned to each integration point, for which a separate finite element computation is performed. From the macroscopic deformation tensor, appropriate boundary conditions may be derived and applied to the RVE at the micro-level. The micro-level computation resolves the local stress/strain fields in the RVE, from which the macroscopic stiffness tensor may be determined, through a suitable homogenisation procedure. The fundamental nature of this approach means that macroscopic constitutive behaviour is not specified and the constitutive behaviour at each material integration point is deduced from the micro-level. This coupled micro-macro approach has already been employed successfully to predict structural behaviour of voided aluminium under pure bending (Kouznetsova et al. 2001) and, thus, could prove suitable to predict behaviour using the micromechanical model developed herein as the micro-level RVE, coupled to a macro-level mesh. As there is obviously a large computational expense associated with such an approach, it is
likely that it could only be implemented in simplified loading situations, using a small micro-level RVE (much smaller than used in this thesis).

The alternative to the coupled micro-macro approach is to determine micro-level response \textit{a priori} and use it to define suitable failure envelopes for the material in three-dimensions, as already discussed. In addition, it is thought that computational micromechanics could be used to enhance understanding and formulation of current continuum damage modelling approaches. The micromechanical model developed herein was shown to predict stiffness reduction and permanent plastic strain in the material under a regime of cyclic loading, all the while capturing actual microscopic damage progression in each of the constituent phases of the composite. Current state-of-the-art continuum damage models (Ladevèze 1992) do not capture such a wide range of behaviour and depend upon non-physical material parameters, such as transverse and shear damage/plasticity coupling factors, to account for non-linear behaviour. The importance of these non-physical coupling factors has received attention lately from O’Higgins \textit{et al.} (2011a, b), however, their physical significance has not been established. It is thus proposed that the micromechanical model be used to investigate the physical significance of such coupling factors, with respect to intra-ply damage mechanisms, by replicating the stress states of both 45° and 67.5° off-axis experimental tests (the tests carried to determine coefficients for these coupling factors). This micromechanical characterisation could help to improve the formulation of the CDM model by considering the fundamental damage mechanisms responsible for non-linear material behaviour. In addition, the CDM approach requires an extensive experimental test series to determine suitable model coefficients. It is thought that, using the virtual testing concept, micromechanical simulations could eventually be used to determine damage development curves for the CDM, using a range of cyclic tensile and shear loading tests, reducing the need for experimental testing. However, such an approach first requires extensive experimental characterisation at the microscale.

\textbf{7.3.2 Microscale Experimental Characterisation}

While the predictive micromechanical modelling capability developed herein has provided novel insights into the formation and growth of microscale damage mechanisms, in order to calibrate some of the model’s input parameters and enhance its
predictions of both local and global material behaviour, a number of microscale experimental tests should be carried out.

Nano-Indentation Testing

High-strength fibre/epoxy composites typically undergo a high temperature curing process in order to consolidate the fibre and matrix phases. The curing process brings about a series of mechanical and chemical changes in the constituent phases. In particular, the matrix phase hardens through a series of chemical reactions which cause it to increase its stiffness and form a chemical bond to the fibres. While bulk properties of both fibre and matrix phases may be obtained with relative ease, their in-situ mechanical behaviour has not been well established. Moreover, it has been previously shown by Hobbiebrunken et al. (2007) that due to the small material volume involved, particularly in inter-fibre regions, the microscale matrix behaviour can be quite sensitive to the size effect, with microscale experimental tests giving quite different results to bulk macroscopic tests. Thus, it is proposed that nano-indentation experiments be carried out on cured composite samples to determine the in-situ mechanical response of the constituent phases. A number of issues raised by the micromechanical study carried out in this thesis could be investigated, such as the effect of local fibre distribution on mechanical response of the matrix phase. Experimental results from composite microscale specimens could be compared to microscale tests carried out on neat resin samples (with no reinforcements). Also, the nano-indentation technique could be used to develop a fibre push-out test in order to characterise the properties of the fibre-matrix interface for use in the three-dimensional micromechanical model.

Microscale Tensile Testing

It is proposed that microscale characterisation be carried out in order to investigate actual formation and growth of intra-ply damage mechanisms in composite laminates. This would be carried out using a micro-tensile tester, placed inside the chamber of a Scanning Electron Microscope (SEM), allowing in-situ observation of how damage initiates and evolves at the microscale. A similar study, in which the material is subject to a range of loading scenarios in the transverse plane, would be carried out in order to validate the performance of the micromechanical model developed herein. In addition, cross-ply laminates could be tested in order to track the
Conclusions and Recommendations

progression of intra-ply damage to the inter-ply region, which would give fascinating insight into the formation of delamination cracks. These in-situ experimental testing techniques coupled with computational micromechanics would facilitate more accurate predictions of local and global deformation mechanisms. This state-of-the-art multi-scale approach to composite design would enhance current empirical and continuum predictive methods, leading to a reduction in experimental phases and more efficient, safe design of composite structures.


References


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References


References


Appendix A

Model Parameter Analysis

A.1 Introduction

This appendix outlines a number of studies carried out to define suitable solution parameters for the micromechanical damage modelling carried out in Chapters 4-6.

A.2 Mesh Sensitivity Analysis

A mesh sensitivity analysis was carried out by considering an RVE, which measured 33×33 µm (i.e. δ=10), to examine the effect of different levels of mesh refinement on the response. For each of the models generated, the level of refinement used was described in terms of variable $n$, which can be defined as the number of elements situated around the circumference of each fibre. Three values of $n$ were examined, where $n=115$, $n=175$ and $n=230$. The resulting discretisation in a region of the RVE which exhibited closely packed fibres is shown in Fig. A.1. In the fibre region, the assumed linear elastic behaviour of the HTA fibres meant that these regions could use a much coarser level of discretisation, allowing for a significant reduction in computational expense for each micromechanical model. Each model was subject to transverse tensile loading, as described in Chapter 4, and had the same interfacial parameters, where $t_{i/s}^0 = 60$ MPa and $\Gamma = 10$ J/m².
Figure A.1: Level of discretisation used in RVE used for the mesh sensitivity analysis.

Figure A.2 shows the resulting transverse tensile response for each value of $n$, where it can be seen that there is a negligible variation in the response for each mesh used (all curves are nearly identical, meaning $n = 230$ is not visible). Figure A.3 shows the final fracture pattern of the RVE for all values of $n$, where the resulting fracture patterns for each mesh are almost identical. It can thus be concluded that a value of $n=115$ can be assumed for the micromechanical analysis, as the results are insensitive to any further mesh refinements.

Figure A.2: Effect of mesh refinement on transverse response.


A.3 Viscosity Co-efficient

The implicit implementation of material models undergoing softening behaviour can lead to severe convergence difficulties. In order to overcome convergence issues, viscous regularisation was used for the cohesive sections (Gao & Bower 2004). This means that ABAQUS allows the stresses to fall outside the limits set by the traction-separation laws governing behaviour at the fibre-matrix interface. This evolution of the viscous stiffness degradation variable can be defined as follows,

\[
\dot{D}_v = \frac{1}{\mu} (D - D_v)
\]  

(A.1)

where \( \mu \) is the viscosity parameter which represents the relaxation time of the viscous system and \( D_v \) is the regularised damage variable. The damaged response of the material is now evaluated using this regularised damage variable such that,

\[
\begin{align*}
  t_n &= \begin{cases} 
  (1-D_v)\tilde{r}_n & t_n \geq 0 \\
  \tilde{r}_n & t_n < 0 
  \end{cases} \\
  t_s &= (1-D_v)\tilde{r}_s
\end{align*}
\]  

(A.2)

To determine a suitable viscosity coefficient for the finite element modelling, a study was carried out using the same RVE outlined in Section A.2. The initial viscosity coefficient chosen for this analysis was \( \mu = 2 \times 10^{-4} \) as it was used by Keane (2009) to investigate fibre-matrix debonding in a periodic hexagonal fibre unit cell. Three other values, of varying orders of magnitude, have been analysed to determine the effect of the viscosity coefficient on the solution. Figure A.4 shows the resulting transverse
response of the models for each viscosity coefficient. It can be seen here that both \( \mu = 2 \times 10^{-2} \) and \( \mu = 2 \times 10^{-3} \) over-predict the transverse strength and fail to accurately capture the response, compared to the lower values. Here, both \( \mu = 2 \times 10^{-4} \) and \( \mu = 2 \times 10^{-5} \) give almost identical responses and it can be thus concluded that a value of \( \mu = 2 \times 10^{-4} \) is a suitable value for use in the micromechanical analysis. It should be noted that for \( \mu = 2 \times 10^{-5} \), the convergence of the model was much slower than \( \mu = 2 \times 10^{-4} \).

![Figure A.4: Effect of viscosity coefficient on the transverse response.](image)

Figure A.4: Effect of viscosity coefficient on the transverse response.
Appendix B

MATLAB and Python Codes

B.1 Introduction

This Appendix contains a number of the MATLAB and Python codes which were described in Chapters 3 and 6. Each of these codes contains comments explaining the structure and purpose of each loop.

B.2 Nearest Neighbour Algorithm

The Nearest Neighbour Algorithm (NNA) (Copyright © 2011 Ted J. Vaughan and Dr. Conor T. McCarthy) was described in Chapter 3 and its function was to generate statistically equivalent fibre distributions for high strength composite materials. The NNA uses 1st and 2nd nearest neighbour distribution functions to define the inter-fibre distances and an experimentally measured diameter distribution function to assign fibre diameters in the RVE. This allows the short range interaction of fibres in the microstructure to be reproduced, enabling an accurate representation of the local microscopic stress state. The following MATLAB code shows the structure of the NNA,
% NEAREST NEIGHBOUR ALGORITHM
% Copyright © 2011 Ted J. Vaughan and Dr. Conor T. McCarthy

% Program Description:
% The Nearest Neighbour Algorithm (NNA) generates statistically equivalent fibre distributions for high strength composite materials using experimentally measured nearest neighbour distribution functions to define the inter-fibre distances and an experimentally measured diameter distribution function to assign fibre diameters in the Representative Volume Element (RVE).

% Further details regarding the NNA may be found at the following source,
% Title: A combined experimental-numerical approach for generating statistically equivalent fibre distributions for high strength laminated composite materials
% Author(s): Vaughan, T. J., McCarthy, C. T.
% Source: Composites Science and Technology
% Volume: 70 Issue: 2 Pages: 291-297 Year: 2010

% Code written by: Ted J. Vaughan

%--------------------------------------------------------------------
% RANDOM NUMBER GENERATOR IS 'RESET' USING THE CLOCK FUNCTION
f1=clock;
rand(f1(1,6));
Vf=0;

% USER ENTERS SIZE OF RVE REQUIRED
Size=input('Enter size of microstructure (in microns) ');

% FIRST FIBRE AND FIBRE RADIUS IS CHOSEN
x(1,1)= (Size)*rand;
y(1,1)= (Size)*rand;
R(1)=lognrnd(Diam_mean,Diam_var)/2;

w=0;
n=1;
A=size(x);

% ALGORITHM IS SET UP ON A 'WHILE' LOOP, AS LONG AS 'n' IS LESS THAN THE SIZE OF THE CENTRE MATRIX, FIBRES CONTINUE TO BE PLACED IN THE REGION.
% THIS MEANS EACH FIBRE IS ASSIGNED A 1ST AND 2ND NEAREST NEIGHBOUR UNTIL THERE IS NO MORE AVAILABLE SPACE IN THE REGION
%--------------------------------------------------------------------
while n<A(1)|n<2;
disp(n)
    count=0;
    A=size(x);
    b=1;
p=0;
q=0;
    while b<A(1);
        if x(b)==-10;
            x(b)=[];
            y(b)=[];
            b=0;
        end
        while q==0;
            while p==0;
                if x(p)==-10;
                    x(p)=[];
                    y(p)=[];
                    p=0;
                end
                p=p+1;
            end
            if x(q)==-10;
                x(q)=[];
                y(q)=[];
                q=0;
            end
            q=q+1;
        end
        b=b+1;
    end
end
R(b)=[ ];
a(b,:)=[ ];
A=size(x);
b=b;

elseif x(b)+5>0;
b=b+1;
end
end
A=size(x);
if n>A(1);
break
end

%INTER-FIBRE DISTANCES ASSIGNED USING LOGISTIC DISTRIBUTIONS FIT TO EXPERIMENTAL

%NEAREST NEIGHBOUR DISTRIBUTION FUNCTIONS
d(A(1)+1)=randraw('logistic',[NND_1mean NND_1var]);
d((A(1)+2))=randraw('logistic',[NND_2mean NND_2var]);

%ANGLES OF ORIENTATION FOR NEIGHBOURING FIBRES ARE CHOSEN
tetha(A(1)+1)=rand*360;
tetha((A(1)+2))=rand*360;

% INDIVIDUAL X AND Y COMPONENTS OF THE DISTANCE VECTOR TO A NEIGHBOURING FIBRE DETERMINED
x0=d(A(1)+1)*(cosd(tetha(A(1)+1)));
y0=d(A(1)+1)*(sind(tetha(A(1)+1)));
x1=d((A(1)+2))*(cosd(tetha((A(1)+2))));
y1=d((A(1)+1+1))*(sind(tetha((A(1)+2))));

%VALUES ADDED TO CURRENT CENTRE POINT GIVING COORDINATES OF NEW NEIGHBOURING FIBRES
x(A(1)+1,1)=x(n,1)+x0;
y(A(1)+1,1)=y(n,1)+y0;
x(A(1)+2,1)=x(n,1)+x1;
y(A(1)+2,1)=y(n,1)+y1;

%RADIUS ASSIGNED TO NEW 1ST NEAREST NEIGHBOURING POINT - CONDITION IS INCLUDED
%SO THAT THE TWO NEIGHBOURING FIBRES CANNOT OVERLAP WITH ONE ANOTHER
R(A(1)+1)=lognrnd(Diam_mean,Diam_var)/2;
c=0;
while R(A(1)+1)−0.1>d(A(1)+1)−R(n);
R(A(1)+1)=lognrnd(Diam_mean,Diam_var)/2;
c=c+1;
if c>100;
d(A(1)+1)=7.13;
tetha(n)=rand*360;
x0=d(n)*(cosd(tetha(n)));
y0=d(n)*(sind(tetha(n)));
x(A(1)+1,1)=x(n,1)+x0;
y(A(1)+1,1)=y(n,1)+y0;
end

%THE POSITION OF THE NEW FIBRE IS NOW CHECKED, ENSURING THAT:
% A) IT LIES WITHIN THE DEFINED AREA OF THE RVE
% B) IT DOES NOT OVERLAP WITH ANY OTHER FIBRES IN THE REGION
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:A(1)+1,A(1)+1);
s=1;
while s<A(1)+1;
\[ \text{dist} = R(s) + R(A(1)+1) + 0.1; \]

\[ R(s); \]

\[ R(A(1)+1); \]

if \[ k(s) > \text{dist} \& x(A(1)+1,1) > 0 \& x(A(1)+1,1) < \text{Size} \& y(A(1)+1,1) > 0 \& y(A(1)+1,1) < \text{Size}; \]

\[ s = s + 1; \]

elseif \[ k(s) < \text{dist} \& x(A(1)+1,1) < 0 \& x(A(1)+1,1) > \text{Size} \& y(A(1)+1,1) < 0 \& y(A(1)+1,1) > \text{Size}; \]

\[ \text{tetha}(n) = \text{rand} \ast 360; \]

\[ x0 = d(n) \ast \cosd(tetha(n)); \]

\[ y0 = d(n) \ast \sind(tetha(n)); \]

\[ x(A(1)+1,1) = x(n,1) + x0; \]

\[ y(A(1)+1,1) = y(n,1) + y0; \]

\[ a = [x \ y]; \]

\[ h = \text{pdist}(a); \]

\[ v = \text{squareform}(h); \]

\[ k = v(1:A(1)+1,A(1)+1); \]

\[ s = 1; \]

\[ \text{count} = \text{count} + 1; \]

if \[ \text{count} > 40 \]

\[ x(A(1)+1,1,1) = -10; \]

\[ y(A(1)+1,1,1) = -10; \]

\[ w = w + 1; \]

break

end

end

% CONDITION TO MAINTAIN A MINIMUM DISTANCE BETWEEN THE FIBRES
% AND THE EDGE OF THE RVE (NOTE: THIS HAS A LARGER INHIBITION
% DISTANCE (0.2um) THAN BETWEEN FIBRES (0.1um) DUE TO THE

\[ \text{REQUIREMENT} \]

% OF OPPOSING NODESETS ON THE RVE TO BE IDENTICAL. THE
% LARGER INHIBITION DISTANCE MITIGATES A LOT OF MESHING
% PROBLEMS WHEN THE MICROSTRUCTURES ARE SUBMITTED TO ABAQUS

if \[ \text{abs}(x(A(1)+1,1) - R(A(1)+1)) < 0.2 || \text{abs}(y(A(1)+1,1) - R(A(1)+1)) < 0.2 \]

\[ \text{R(A(1)+1)) < 0.2 || \text{abs}((\text{Size} - x(A(1)+1,1)) - R(A(1)+1)) < 0.2 || \text{abs}((\text{Size} - y(A(1)+1,1)) - R(A(1)+1)) < 0.2 \]

\[ \text{tetha}(n) = \text{rand} \ast 360; \]

\[ x0 = d(n) \ast \cosd(tetha(n)); \]

\[ y0 = d(n) \ast \sind(tetha(n)); \]

\[ x(A(1)+1,1) = x(n,1) + x0; \]

\[ y(A(1)+1,1) = y(n,1) + y0; \]

\[ a = [x \ y]; \]

\[ h = \text{pdist}(a); \]

\[ v = \text{squareform}(h); \]

\[ k = v(1:A(1)+1,A(1)+1); \]

\[ s = 1; \]

\[ \text{count} = \text{count} + 1; \]

if \[ \text{count} > 40 \]

\[ x(A(1)+1,1,1) = -10; \]

\[ y(A(1)+1,1,1) = -10; \]

\[ w = w + 1; \]

break

end

end

% RADIUS ASSIGNED TO NEW 2ND NEAREST NEIGHBOURING POINT – CONDITION IS

INCLUDED

% SO THAT THE TWO NEIGHBOURING FIBRES CANNOT OVERLAP WITH ONE
% ANOTHER, AS BEFORE

\[ R(A(1)+2) = \lognrnd(Diam\_mean,Diam\_var)/2; \]

while \[ R(A(1)+2) - 0.1 > d(A(1)+1+1) - R(n); \]

\[ R(A(1)+2) = \lognrnd(Diam\_mean,Diam\_var)/2; \]

\[ c = c + 1; \]

if \[ c > 100; \]

\[ d(A(1)+2) = 7.27; \]

\[ \text{tetha}(A(1)+2) = \text{rand} \ast 360; \]
\[ x_1 = d(A(1) + 2) \cdot \cos(\theta(n)); \]
\[ y_1 = d(A(1) + 2) \cdot \sin(\theta(n)); \]
\[ x((A(1) + 2), 1) = x(n, 1) + x_1; \]
\[ y((A(1) + 2), 1) = y(n, 1) + y_1; \]

\% \% THE POSITION OF THE NEW 2nd NEAREST NEIGHBOUR IS NOW CHECKED, ENSURING THAT:
\% A) IT LIES WITHIN THE DEFINED AREA OF THE RVE
\% B) IT DOES NOT OVERLAP WITH ANY OTHER FIBRES IN THE REGION
\% C) IT MEETS THE REQUIREMENT OF THE MINDISTANCE BETWEEN THE FIBRES AND THE EDGE OF THE RVE
\%

\% CONDITION TO MAINTAIN A MINIMUM DISTANCE BETWEEN THE FIBRES
\% AND THE EDGE OF THE RVE (NOTE: THIS HAS A LARGER INHIBITION DISTANCE (0.2um) THAN BETWEEN FIBRES (0.1um) DUE TO THE REQUIREMENT
\% OF OPPOSING NODESETS ON THE RVE TO BE IDENTICAL

\% OF OPPOSING NODESETS ON THE RVE TO BE IDENTICAL
\% IF \( \text{abs}(x(A(1) + 2, 1) - R(A(1) + 2)) < 0.2 \) AND \( \text{abs}(y(A(1) + 2, 1) - R(A(1) + 2)) < 0.2 \)
\% \( \text{abs}((\text{Size} - x(A(1) + 2, 1)) - R(A(1) + 2)) < 0.2 \) AND \( \text{abs}((\text{Size} - y(A(1) + 2, 1)) - R(A(1) + 2)) < 0.2 \)
\%

\% THE POSITION OF THE NEW 2nd NEAREST NEIGHBOUR IS NOW CHECKED, ENSURING THAT:
\% A) IT LIES WITHIN THE DEFINED AREA OF THE RVE
\% B) IT DOES NOT OVERLAP WITH ANY OTHER FIBRES IN THE REGION
\% C) IT MEETS THE REQUIREMENT OF THE MINDISTANCE BETWEEN THE FIBRES AND THE EDGE OF THE RVE (NOTE: THIS HAS A LARGER INHIBITION DISTANCE (0.2um) THAN BETWEEN FIBRES (0.1um) DUE TO THE REQUIREMENT
\% OF OPPOSING NODESETS ON THE RVE TO BE IDENTICAL
%THE NEXT SERIES OF LOOPS ARE TO ENSURE THAT THE RVEs GENERATED
%GEOMETRICALLY PERIODIC. THIS MEANS THAT FOR ANY FIBRE CROSSING A BOUNDARY
%OF THE RVE, A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE.
%NUMEROUS CHECKS ARE CARRIED OUT TO ENSURE NO OVERLAPS OCCUR DURING THIS
%PROCEDURE

l=0;
if  Size-x(A(1)+1,1)<R(A(1)+1)&x(A(1)+1,1)<Size
x(A(1)+(l+3),1)=x(A(1)+1,1)-Size;
y(A(1)+(l+3),1)=y(A(1)+1,1);
R(A(1)+(l+3))=R(A(1)+1);
p=1;
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
dist=R(s)+R((A(1)+(l+3)));
if k(s)>dist+0.1;
s=s+1;
elseif k(s)<dist+0.1;
x(s,1)=-10;
y(s,1)=-10;
s=s+1;
end
l=l+1;
end

if x(A(1)+1,1)<R(A(1)+1)&x(A(1)+1,1)>0
x(A(1)+(l+3),1)=x(A(1)+1,1)+Size;
y(A(1)+(l+3),1)=y(A(1)+1,1);
R(A(1)+(l+3))=R(A(1)+1);
p=1;
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
dist=R(s)+R((A(1)+(l+3)));
if k(s)>dist+0.1;
s=s+1;
elseif k(s)<dist+0.1;
x(s,1)=-10;
y(s,1)=-10;
s=s+1;
end
l=l+1;
end

if Size-y(A(1)+1,1)<R(A(1)+1)&y(A(1)+1,1)<Size
y(A(1)+(l+3),1)=y(A(1)+1,1)-Size;
x(A(1)+(l+3),1)=x(A(1)+1,1);
R(A(1)+(l+3))=R(A(1)+1);
q=1;
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
    dist=R(s)+R((A(1)+(l+3)))+0.1;
    if k(s)>dist;
        s=s+1;
    elseif k(s)<dist;
        x(s,1)=-10;
        y(s,1)=-10;
        s=s+1;
    end
end
l=l+1;
end
if y(A(1)+1,1)<R(A(1)+1)&y(A(1)+1,1)>0
    y(A(1)+(l+3),1)=y(A(1)+1,1)+Size;
    x(A(1)+(l+3),1)=x(A(1)+1,1);
    R(A(1)+(l+3))=R(A(1)+1);
    q=1;
    a=[x y];
    h=pdist(a);
    v=squareform(h);
    k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
    s=1;
    while s<(A(1)+(l+3));
        dist=R(s)+R((A(1)+(l+3)))+0.1;
        if k(s)>dist;
            s=s+1;
        elseif k(s)<dist;
            x(s,1)=-10;
            y(s,1)=-10;
            s=s+1;
        end
    end
    l=l+1;
end
if x(A(1)+2,1)<R(A(1)+2)&x(A(1)+2,1)>0
    x(A(1)+(l+3),1)=x(A(1)+2,1)+Size;
    y(A(1)+(l+3),1)=y(A(1)+2,1);
    R(A(1)+(l+3))=R(A(1)+2);
    a=[x y];
    h=pdist(a);
    v=squareform(h);
    k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
    s=1;
    while s<(A(1)+(l+3));
        dist=R(s)+R((A(1)+(l+3)))+0.1;
        if k(s)>dist;
            s=s+1;
        elseif k(s)<dist;
            x(s,1)=-10;
            y(s,1)=-10;
            s=s+1;
        end
    end
    l=l+1;
end
if Size-x(A(1)+2,1)<R(A(1)+2)&x(A(1)+2,1)<Size
    x(A(1)+(l+3),1)=x(A(1)+2,1)-Size;
    y(A(1)+(l+3),1)=y(A(1)+2,1);
    R(A(1)+(l+3))=R(A(1)+2);
    a=[x y];
    h=pdist(a);
    v=squareform(h)

Appendix B
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));  
s=1;

while s<(A(1)+(l+3));
    dist=R(s)+R((A(1)+(l+3)))+0.1;
    if k(s)>dist;
        s=s+1;
    elseif k(s)<dist;
        x(s,1)=-10;
        y(s,1)=-10;
        s=s+1;
    end
end
l=l+1;
end

if y(A(1)+2,1)<R(A(1)+2)&y(A(1)+2,1)>0
    y(A(1)+(l+3),1)=y(A(1)+2,1)+Size;
    x(A(1)+(l+3),1)=x(A(1)+2,1);
    R(A(1)+(l+3))=R(A(1)+2);
    a=[x y];
    h=pdist(a);
    v=squareform(h);
    k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
    s=1;

    while s<(A(1)+(l+3));
        dist=R(s)+R((A(1)+(l+3)))+0.1;
        if k(s)>dist;
            s=s+1;
        elseif k(s)<dist;
            x(s,1)=-10;
            y(s,1)=-10;
            s=s+1;
        end
    end
l=l+1;
end

if Size-y(A(1)+2,1)<R(A(1)+2)&y(A(1)+2,1)<Size
    y(A(1)+(l+3),1)=y(A(1)+2,1)-Size;
    x(A(1)+(l+3),1)=x(A(1)+2,1);
    R(A(1)+(l+3))=R(A(1)+2);
    a=[x y];
    h=pdist(a);
    v=squareform(h);
    k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
    s=1;

    while s<(A(1)+(l+3));
        dist=R(s)+R((A(1)+(l+3)))+0.1;
        if k(s)>dist;
            s=s+1;
        elseif k(s)<dist;
            x(s,1)=-10;
            y(s,1)=-10;
            s=s+1;
        end
    end
l=l+1;
end

if x(A(1)+1,1)<R(A(1)+1)&x(A(1)+1,1)>0&y(A(1)+1,1)<R(A(1)+1)&y(A(1)+1,1)>0
    x(A(1)+(l+3),1)=x(A(1)+1,1)+Size;
    y(A(1)+(l+3),1)=y(A(1)+1,1)+Size;
    R(A(1)+(l+3))=R(A(1)+1);
    p=1;
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
dist=R(s)+R((A(1)+(l+3)));
if k(s)>dist+0.1;
s=s+1;
elseif k(s)<dist+0.1;
x(s,1)=-10;
y(s,1)=-10;
s=s+1;
end
end
l=l+1;
end
if x(A(1)+2,1)<R(A(1)+2)\&x(A(1)+2,1)>0\&y(A(1)+2,1)<R(A(1)+2)\&y(A(1)+2,1)>0
x(A(1)+(l+3),1)=x(A(1)+2,1)+Size;
y(A(1)+(l+3),1)=y(A(1)+2,1)+Size;
R(A(1)+(l+3))=R(A(1)+2);
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
dist=R(s)+R((A(1)+(l+3)))+0.1;
if k(s)>dist;
s=s+1;
elseif k(s)<dist;
x(s,1)=-10;
y(s,1)=-10;
s=s+1;
end
end
l=l+1;
end
if Size-
x(A(1)+1,1)<R(A(1)+1)\&x(A(1)+1,1)<Size\&y(A(1)+1,1)<R(A(1)+1)\&y(A(1)+1,1)>0;
x(A(1)+(l+3),1)=x(A(1)+1,1)-Size;
y(A(1)+(l+3),1)=y(A(1)+1,1)+Size;
R(A(1)+(l+3))=R(A(1)+1);
p=1;
a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
dist=R(s)+R((A(1)+(l+3)));
if k(s)>dist+0.1;
s=s+1;
elseif k(s)<dist+0.1;
x(s,1)=-10;
y(s,1)=-10;
s=s+1;
end
end
l=l+1;
end
if Size-
x(A(1)+2,1)<R(A(1)+2)\&x(A(1)+2,1)<Size\&y(A(1)+2,1)<R(A(1)+2)\&y(A(1)+2,1)>0;
x(A(1)+(l+3),1)=x(A(1)+2,1)-Size;
\[
y(A(1)+(l+3),1) = y(A(1)+2,1) + \text{Size};
\]
\[
R(A(1)+(l+3)) = R(A(1)+2);
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:(A(1)+(l+3)),(A(1)+(l+3)));
\]
\[
s = 1;
\]
\[
\text{while } s < (A(1)+(l+3));
\]
\[
\text{dist} = R(s) + R((A(1)+(l+3))) + 0.1;
\]
\[
\text{if } k(s) > \text{dist};
\]
\[
s = s + 1;
\]
\[
\text{elseif } k(s) < \text{dist};
\]
\[
x(s,1) = -10;
\]
\[
y(s,1) = -10;
\]
\[
s = s + 1;
\]
\[
\end
\]
\[
l = l + 1;
\]
\[
\end
\]
\[
\text{if } \text{Size} - y(A(1)+1,1) < R(A(1)+1) \& y(A(1)+1,1) < \text{Size} \& x(A(1)+1,1) < R(A(1)+1) \& x(A(1)+1,1) > 0
\]
\[
y(A(1)+(l+3),1) = y(A(1)+1,1) - \text{Size};
\]
\[
x(A(1)+(l+3),1) = x(A(1)+1,1) + \text{Size};
\]
\[
R(A(1)+(l+3)) = R(A(1)+1);
\]
\[
q = 1;
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:(A(1)+(l+3)),(A(1)+(l+3)));
\]
\[
s = 1;
\]
\[
\text{while } s < (A(1)+(l+3));
\]
\[
\text{dist} = R(s) + R((A(1)+(l+3))) + 0.1;
\]
\[
\text{if } k(s) > \text{dist};
\]
\[
s = s + 1;
\]
\[
\text{elseif } k(s) < \text{dist};
\]
\[
x(s,1) = -10;
\]
\[
y(s,1) = -10;
\]
\[
s = s + 1;
\]
\[
\end
\]
\[
l = l + 1;
\]
\[
\end
\]
\[
\text{if } \text{Size} - y(A(1)+2,1) < R(A(1)+2) \& y(A(1)+2,1) < \text{Size} \& x(A(1)+2,1) < R(A(1)+2) \& x(A(1)+2,1) > 0
\]
\[
y(A(1)+(l+3),1) = y(A(1)+2,1) - \text{Size};
\]
\[
x(A(1)+(l+3),1) = x(A(1)+2,1) + \text{Size};
\]
\[
R(A(1)+(l+3)) = R(A(1)+2);
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:(A(1)+(l+3)),(A(1)+(l+3)));
\]
\[
s = 1;
\]
\[
\text{while } s < (A(1)+(l+3));
\]
\[
\text{dist} = R(s) + R((A(1)+(l+3))) + 0.1;
\]
\[
\text{if } k(s) > \text{dist};
\]
\[
s = s + 1;
\]
\[
\text{elseif } k(s) < \text{dist};
\]
\[
x(s,1) = -10;
\]
\[
y(s,1) = -10;
\]
\[
s = s + 1;
\]
\[
\end
\]
\[
l = l + 1;
\]
\[
\end
\]
if Size-y(A(1)+1,1)<R(A(1)+1)&y(A(1)+1,1)<Size & x(A(1)+1,1)<R(A(1)+1)&x(A(1)+1,1)<Size;
y(A(1)+(l+3),1)=y(A(1)+1,1)-Size;
x(A(1)+(l+3),1)=x(A(1)+1,1)-Size;
R(A(1)+(l+3))=R(A(1)+1);
q=1;

a=[x y];
h=pdist(a);
v=squareform(h);
k=v(1:(A(1)+(l+3)),(A(1)+(l+3)));
s=1;
while s<(A(1)+(l+3));
    dist=R(s)+R((A(1)+(l+3)))+0.1;
    if k(s)>dist;
        s=s+1;
    elseif k(s)<dist;
        x(s,1)=-10;
        y(s,1)=-10;
        s=s+1;
    end
end
l=l+1;
end

if Size-y(A(1)+2,1)<R(A(1)+2)&y(A(1)+2,1)<Size & x(A(1)+2,1)<R(A(1)+2)&x(A(1)+2,1)<Size;
y(A(1)+(l+3),1)=y(A(1)+2,1)-Size;
x(A(1)+(l+3),1)=x(A(1)+2,1)-Size;
R(A(1)+(l+3))=R(A(1)+2);

%-------------------------------------------------------------------------
n=n+1  ;
A=size(x);
end

x(A(1))=[];
y(A(1))=[];
R(A(1))=[];
a(A(1),:)=[];

%-------------------------------------------------------------------------

%THE FOLLOWING LOOP PLOTS THE RESULTING NUMERICAL MICROSTRUCTURE ON A GRAPH
M=256;
t=(0:M)*2*pi/M;
hold off
for z=1:(A(1)-1)%
    plot(R(z)*cos(t)+a(z,1),R(z)*sin(t)+a(z,2),'k');
    hold on;
    p=R(z)*cos(t)+a(z,1);
    q=R(z)*sin(t)+a(z,2);
end

hold on
B.3 Hard-Core Model

As discussed in Chapter 2, the HCM has been widely used to generate lower fibre volume fraction microstructures (less than approximately $V_f = 50\%$) for composite materials. Random sequential adsorption is used to generate the Hard-Core arrangement, whereby the simulation process sequentially places fibres in random positions within the domain. If a newly deposited fibre overlaps with any pre-existing fibre, it is rejected and a new random centre position is generated. Once the fibre does not overlap with any pre-existing fibres, its position is fixed and does not move. The process is repeated until the model reaches the desired fibre volume fraction (which is
specified by the user) or reaches its jamming limit which is in the region of 54% fibre volume fraction.

```matlab
%% HARD-CORE MODEL

Program Description:
The program generates fibre distribution conforming to the Hard-Core Model (HCM), which is series of fibres randomly distributed within a square region (RVE). The size of the region and the desired fibre volume fraction are defined by the user.

% NOTE: There is an upper limit on the fibre volume fraction of ~54% due to the inherent constraints of the HCM.

% THE SIZE OF THE RVE AND DESIRED FIBRE VOLUME FRACTION ARE ENTERED BY THE USER
Size=input('Enter size of RVE ')
Vf1=input('Enter desired Volume fraction ')

% RANDOM NUMBER GENERATOR IS 'RESET' USING THE CLOCK FUNCTION
f1=clock;
rand(f1(1,6));
Vf=0;

% A NUMBER OF VARIABLES ARE INITIALISED
M=256;
t=(0:M)*2*pi/M;
Vf=0;
area=0;

% THE FIRST POINT IN ASSIGNED USING THE RANDOM NUMBER GENERATOR. NOTE: FOR THE HCM THE FIBRE RADIUS IS CONSTANT, IN THIS CASE r=3.3.
r=3.3;
x(1,1)=rand*(Size-2*r)+r;
y(1,1)=rand*(Size-2*r)+r;
s=2;
e=0;

% ALGORITHM IS SET UP ON A 'WHILE' LOOP, AS LONG AS 'n' THE CURRENT VOLUME FRACTION (Vf) IS LESS THAN THE DESIRED VOLUME FRACTION (Vf1), THE PROGRAM CONTINUES TO PLACE FIBRES IN THE RVE
while (Vf<=Vf1)

% NEW FIBRES ASSIGNED RANDOM POSITIONS IN THE RVE
    x(s,1)=rand*(Size);
    y(s,1)=rand*(Size);
    a=[x y];

% DETERMINE A DISTANCE MATRIX FOR ALL FIBRES IN THE RVE
    h=pdist(a);
    v=squareform(h);
    k=v(1:s,s);
```
d=1;

% THIS LOOP ENSURES THAT THE NEWLY PLACED FIBRES DO NOT OVERLAP WITH
PREVIOUSLY DEPOSITED FIBRES. IF AN OVERLAP OCCURS, THE NEW FIBRE IS ASSIGNED
NEW RANDOM POSITIONS UNTIL A SUITABLE CONFIGURATION CAN BE FOUND.

while d<s;
    if k(d)>0.1+r+r
        d=d+1;
    elseif k(d)<0.1+r+r
        x(s,1)=rand*(Size);
        y(s,1)=rand*(Size);
        a=[x y];
        h=pdist(a);
        u=sort(h);
        v=squareform(h);
        k=v(1:s,s);
        d=1;
        e=e+1;
    end
end

% THE LOOP IS BROKEN AFTER ‘X’ AMOUNT OF ITERATIONS, WHICH SIGNIFIES THE HCM
HAS REACHED ITS JAMMING LIMIT (~54%)

if e>1e04;,
    b=length(a);
    a(b,:)=[];
    x(b)=[];
    y(b)=[];
    break, end
end

% THE NEXT SERIES OF LOOPS ARE TO ENSURE THAT THE RVEs GENERATED
% GEOMETRICALLY PERIODIC. THIS MEANS THAT FOR ANY FIBRE CROSSING A BOUNDARY
% OF THE RVE, A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE.
% NUMEROUS CHECKS ARE CARRIED OUT TO ENSURE NO OVERLAPS OCCUR DURING THIS
% PROCEDURE

% IF FIBRE CROSSES LEFT EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING
% FACE SHOULD THERE BE SPACE AVAILABLE FOR IT

if x(s,1)<r&x(s,1)>0&y(s,1)>r&y(s,1)<(Size-r)
    x(s+1,1)=x(s,1)+Size;
    y(s+1,1)=y(s,1);
    p=1;
    a=[x y];
    h=pdist(a);
    v=squareform(h);
    k=v(l:s+1,(s+1));
    h=1;
    while h<s;
        dist=2*r;
        if k(h)>dist+0.1;
            h=h+1;
        elseif k(h)<dist+0.1;
            x(s)=[ ];
            y(s)=[ ];
            a=[x y];
        end
end

% IF FIBRE CROSSES LEFT EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING
% FACE SHOULD THERE BE SPACE AVAILABLE FOR IT
Appendix B

\[
s = s-2;
break
end
\]

end

\[
s = s+1;
\]

end

% IF FIBRE PENETRATES RIGHT EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE SHOULD THERE BE SPACE AVAILABLE FOR IT

\[
\text{if } x(s,1) > (\text{Size}-r) \& x(s,1) < \text{Size} \& y(s,1) > r \& y(s,1) < (\text{Size}-r) \]
\[
x(s+1,1) = x(s,1) - \text{Size};
\]
\[
y(s+1,1) = y(s,1);
\]
\[
p = 1;
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:s+1,(s+1));
\]
\[
h = 1;
\]
\[
\text{while } h < (s);
\]
\[
dist = 2*r;
\]
\[
\text{if } k(h) > \text{dist} + 0.1;
\]
\[
h = h + 1;
\]
\[
\text{elseif } k(h) < \text{dist} + 0.1;
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
a = [x \ y];
\]
\[
s = s-2;
\]
\[
break
\]
\end
\]

\end

% IF FIBRE PENETRATES BOTTOM EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE SHOULD THERE BE SPACE AVAILABLE FOR IT

\[
\text{if } y(s,1) < r \& y(s,1) > 0 \& x(s,1) > r \& x(s,1) < (\text{Size}-r) \]
\[
x(s+1,1) = x(s,1);
\]
\[
y(s+1,1) = y(s,1) + \text{Size};
\]
\[
p = 1;
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:s+1,(s+1));
\]
\[
h = 1;
\]
\[
\text{while } h < (s);
\]
\[
dist = 2*r;
\]
\[
\text{if } k(h) > \text{dist} + 0.1;
\]
\[
h = h + 1;
\]
\[
\text{elseif } k(h) < \text{dist} + 0.1;
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
a = [x \ y];
\]
\[
s = s-2;
\]
\[
break
\]
\end
\]

\end

% IF FIBRE PENETRATES TOP EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE SHOULD THERE BE SPACE AVAILABLE FOR IT

\[
\text{if } y(s,1) < 0 \& y(s,1) > r \& x(s,1) > r \& x(s,1) < (\text{Size}-r) \]
\[
x(s+1,1) = x(s,1) - \text{Size};
\]
\[
y(s+1,1) = y(s,1);
\]
\[
p = 1;
\]
\[
a = [x \ y];
\]
\[
h = \text{pdist}(a);
\]
\[
v = \text{squareform}(h);
\]
\[
k = v(1:s+1,(s+1));
\]
\[
h = 1;
\]
\[
\text{while } h < (s);
\]
\[
dist = 2*r;
\]
\[
\text{if } k(h) > \text{dist} + 0.1;
\]
\[
h = h + 1;
\]
\[
\text{elseif } k(h) < \text{dist} + 0.1;
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
x(s) = [];
\]
\[
y(s) = [];
\]
\[
a = [x \ y];
\]
\[
s = s-2;
\]
\[
break
\]
\end
\]

\end

% IF FIBRE PENETRATES TOP EDGE A CORRESPONDING FIBRE IS PLACED ON THE OPPOSING FACE SHOULD THERE BE SPACE AVAILABLE FOR IT
if \( y(s,1) > (\text{Size}-r) \land y(s,1) < \text{Size} \land x(s,1) > r \land x(s,1) < (\text{Size}-r) \)

\[
x(s+1,1) = x(s,1);
y(s+1,1) = y(s,1) - \text{Size};\]

\[p = 1;\]
\[a = [x \ y];\]
\[h = \text{pdist}(a);\]
\[v = \text{squareform}(h);\]
\[x = v(1:s+1, (s+1));\]
\[h = 1;\]

while \( h < (s) \)

\[\text{dist} = 2 \times r;\]
\[\text{if } k(h) > \text{dist} + 0.1;\]

\[h = h + 1;\]
\[\text{elseif } k(h) < \text{dist} + 0.1;\]

\[x(s) = [];\]
\[y(s) = [];\]

\[a = [x \ y];\]
\[s = s - 2;\]

break;

\[s = s + 1;\]
end

% IN THIS VERSION THE CORNER FIBRES ARE EXCLUDED FOR SIMPLICITY

if \( x(s,1) < r \land x(s,1) > 0 \land y(s,1) < r \land y(s,1) > 0 \)

\[x(s) = [];\]
\[y(s) = [];\]
\[a = [x \ y];\]
\[s = s - 1;\]
end

if \( x(s,1) < r \land x(s,1) > 0 \land y(s,1) > (\text{Size}-r) \land y(s,1) > 0 \)

\[x(s) = [];\]
\[y(s) = [];\]
\[a = [x \ y];\]
\[s = s - 1;\] if \( x(s,1) > (\text{Size}-r) \land x(s,1) < \text{Size} \land y(s,1) > (\text{Size}-r) \land y(s,1) < \text{Size} \)

\[x(s) = [];\]
\[y(s) = [];\]
\[a = [x \ y];\]
\[s = s - 1;\] if \( x(s,1) > (\text{Size}-r) \land x(s,1) < \text{Size} \land y(s,1) < r \land y(s,1) > 0 \)

\[x(s) = [];\]
\[y(s) = [];\]
\[a = [x \ y];\]
\[s = s - 1;\]
end

\[
\% \text{CALCULATE THE CURRENT FIBRE VOLUME FRACTION (Vf)}
\]
\[s = s + 1;\]

area = 0;
da = size(a);
for \( i = 1:d(1,1) \)

\[\text{if } x(i) > 0 \land x(i) < \text{Size} \land y(i) > 0 \land y(i) < \text{Size};\]

\[\text{area} = (\pi) \times (r)^2 \times \text{area};\]

end

\[\text{Vf} = (100 \times \text{area} / (\text{Size}^2));\]
end
b=length(a);
Vf=Vf

%-------------------------------------------------------------------------
%THE FOLLOWING LOOP PLOTS THE RESULTING NUMERICAL MICROSTRUCTURE ON A GRAPH

for z=1:b
    plot(r*cos(t)+x(z),r*sin(t)+y(z));
    hold on
    plot(x,y,'+')
    axis([0 Size 0 Size])%Shows the axes limits in the form axis([xmin xmax ymin ymax zmin zmax])
    axis square
end
hold off

%-------------------------------------------------------------------------
%PASS A NUMBER OF VARIABLES FOR SUBSEQUENT CODES
R(1:length(a),1)=r;
NNAradius=R;
NNAcentre=a;
NNASize=Size;

%-------------------------------------------------------------------------

B.4 Python Script to interface between MATLAB and ABAQUS

The following is a Python Script which would have been generated by the
COMM Toolbox and subsequently used to create an ABAQUS Input File of an RVE
which has been generated. This Python script is a series of commands which, when
executed by the ABAQUS Python Interpreter, can create/modify components of an
ABAQUS finite element model.

```python
#% PYTHON GENERATOR

#Program Description:
#This program generates an ABAQUS finite element model of an RVE created by
either the NNA or HCM.

#% PYTHON OBJECTS IMPORTED TO WORKSPACE

from abaqus import *
from abaqusConstants import *
mdb.models.changeKey(fromName='Model-1', toName='microstructure')
s=mdb.models['microstructure'].ConstrainedSketch(name='microprofile',
    sheetSize=400)
g, v, d, c = s.geometry, s.vertices, s.dimensions, s.constraints

# INITIAL SKETCH FOR OUTER RVE BOUNDARIES IS DRAWN
s.sketchOptions.setValues(decimalPlaces=3)
s.setPrimaryObject(option=STANDALONE)
```
n = mdb.models['microstructure'].ConstrainedSketch(name='microprofile_area', sheetSize=400)
g, v, d, c = n.geometry, n.vertices, n.dimensions, n.constraints
n.rectangle(point1=(0, 0), point2=(20.0000000000, 20.0000000000))
p = mdb.models['microstructure'].Part(name='RVE', dimensionality=TWO_D_PLANAR, type=DEFORMABLE_BODY)
p = mdb.models['microstructure'].parts['RVE']
p.BaseShell(sketch=n)

%% SKETCH WITH FIBRE POSITIONS IS DRAWN
s.CircleByCenterPerimeter(center=(5.9372776484, 10.2813386144),
   point1=(8.9944874608, 10.2813386144))
s.CircleByCenterPerimeter(center=(16.2615885923, 13.6809432115),
   point1=(19.6166817820, 13.6809432115))
s.CircleByCenterPerimeter(center=(2.6835320578, 4.0095107796),
   point1=(6.0670222263, 4.0095107796))
s.CircleByCenterPerimeter(center=(2.4411921598, 16.1395981837),
   point1=(5.5819145753, 16.1395981837))
s.CircleByCenterPerimeter(center=(22.6835320578, 4.0095107796),
   point1=(26.0670222263, 4.0095107796))
s.CircleByCenterPerimeter(center=(22.4411921598, 16.1395981837),
   point1=(25.5819145753, 16.1395981837))
s.CircleByCenterPerimeter(center=(15.2543886105, 6.7055049126),
   point1=(18.8003174817, 6.7055049126))
s.CircleByCenterPerimeter(center=(9.0347705227, 0.7671220193),
   point1=(12.3984630946, 0.7671220193))
s.CircleByCenterPerimeter(center=(9.0347705227, 20.7671220193),
   point1=(12.3984630946, 20.7671220193))
Faces = p.faces
mainface = Faces.findAt([(1, 1, 0)])

%% PARTITION THE PLANAR BODY WITH THE SKETCH OF THE FIBRES
p.PartitionFaceBySketch(faces=mainface, sketch=s)

%% MATERIALS ARE CREATED AND ASSIGNED PROPERTIES
mdb.models['microstructure'].Material('Fibre')
mdb.models['microstructure'].materials['Fibre'].Elastic(table=((28.0E9, 0.27), ))
mdb.models['microstructure'].Material('Matrix')
mdb.models['microstructure'].materials['Matrix'].Elastic(table=((3.68E9, 0.34), ))

% FIBRE AND MATRIX SECTIONS ARE CREATED AND AN ORIENTATION SYSTEM DEFINED
mdb.models['microstructure'].HomogeneousSolidSection(name='Matrix Section', material='Matrix', thickness=1.0)
mdb.models['microstructure'].HomogeneousSolidSection(name='Fibre Section', material='Fibre', thickness=1.0)
import regionToolset
datums = p.DatumCsysByThreePoints(name='Datum csys-1', coordSysType=CARTESIAN, origin=(0.0, 0.0, 0.0), point1=(1.0, 0.0, 0.0), point2=(0.0, 1.0, 0.0))

% FIBRE AND MATRIX REGIONS ASSIGNED SECTION PROPERTIES, MATERIAL ORIENTATIONS AND MESH CONTROLS (CARRIED OUT INDIVIDUALLY FOR EACH FIBRE IN THE MICROSTRUCTURE

% Fibre 1
F = p.faces
faces = F.findAt(((8.9954874608, 10.2813386144, 0.0), ))
region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Matrix Section', offset=0.0)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)
elemType1 = mesh.ElemType(elemCode=CPE3, elemLibrary=STANDARD)
pickedRegions = (faces, )
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% Fibre 2
faces = F.findAt(((5.9372776484, 10.2813386144, 0.0), ))
region = regionToolset.Region(faces=faces)
p.setSectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.setMaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)

% Fibre 3
faces = F.findAt(((16.2615885923, 13.6809432115, 0.0), ))
region = regionToolset.Region(faces=faces)
p.setSectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.setMaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)

% Fibre 4
faces = F.findAt(((2.6835320578, 4.0095107796, 0.0), ))
region = regionToolset.Region(faces=faces)
p.setSectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.setMaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)

% Fibre 5
faces = F.findAt(((2.4411921598, 16.1395981837, 0.0), ))
region = regionToolset.Region(faces=faces)
p.setSectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.setMaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)

% Fibre 6
faces = F.findAt(((19.9999000000, 4.0095107796, 0.0), ))
Appendix B

region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.MaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)
elemType1 = mesh.ElemType(elemCode=CPE3, elemLibrary=STANDARD)
pickedRegions = (faces, )
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% Fibre 7
faces = F.findAt(((19.9999000000, 16.1395981837, 0.0), ))
region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.MaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)
elemType1 = mesh.ElemType(elemCode=CPE3, elemLibrary=STANDARD)
pickedRegions = (faces, )
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% Fibre 8
faces = F.findAt(((15.2543886105, 6.7055049126, 0.0), ))
region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.MaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)
elemType1 = mesh.ElemType(elemCode=CPE3, elemLibrary=STANDARD)
pickedRegions = (faces, )
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% Fibre 9
faces = F.findAt(((9.0347705227, 0.7671220193, 0.0), ))
region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.MaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)
elemType1 = mesh.ElemType(elemCode=CPE3, elemLibrary=STANDARD)
pickedRegions = (faces, )
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% Fibre 10
faces = F.findAt(((9.0347705227, 19.9999000000, 0.0), ))
region = regionToolset.Region(faces=faces)
p.SectionAssignment(region=region, sectionName='Fibre Section', offset=0.0)
datums = p.datums[3]
p.MaterialOrientation(region=region, orientationType=SYSTEM, localCsys=datums)
f = p.faces
pickedRegions = f
import mesh
p.setMeshControls(regions=pickedRegions, elemShape=TRI)

pickedRegions = (faces,)
p.setElementType(regions=pickedRegions, elemTypes=(elemType1,))

% RESET THE DISPLAY OPTIONS (FOR ABAQUS/CAR USE)
s.unsetPrimaryObject()
session.viewports['Viewport: 1'].setValues(displayedObject=p)
session.viewports['Viewport: 1'].partDisplay.setValues(sectionAssignments=ON,
  engineeringFeatures=ON)
a = mdb.models['microstructure'].rootAssembly
a.DatumCsysByDefault(CARTESIAN)

mdb.models['microstructure'].StaticStep(name='Apply Displacement',
  previous='Initial', description='Apply surface displacement')
session.viewports['Viewport: 1'].assemblyDisplay.setValues(step='Apply
  Displacement')
p = mdb.models['microstructure'].parts['RVE']
f = p.faces

% GLOBAL SEEDING DEFINITIONS DEFINED AND SUBSEQUENTLY MESHED

p = mdb.models['microstructure'].parts['RVE']
p.seedPart(size=0.6, deviationFactor=0.1)
p = mdb.models['microstructure'].parts['RVE']
p.generateMesh()

% JOB FILES CREATED

mdb.Job(name='e22', model='microstructure', description='e22')
mdb.Job(name='g23', model='microstructure', description='g23')
mdb.Job(name='e33', model='microstructure', description='e33')

%INPUT FILES WRITTEN TO WORKSPACE

mdb.jobs['e22'].writeInput(consistencyChecking=OFF)
mdb.jobs['e33'].writeInput(consistencyChecking=OFF)
mdb.jobs['g23'].writeInput(consistencyChecking=OFF)