In-situ X-ray Computed Tomography Tests and Numerical Modelling of Ultra High Performance Fibre Reinforced Concrete

A THESIS

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Abstract

Ultra high performance fibre reinforced concrete (UHPFRC) is a relatively new fibre reinforced cementitious composite and has become very popular in construction applications. Extensive experimental studies have been conducted, demonstrating its superior properties such as much higher strength, ductility and durability than conventional fibre reinforced concrete (FRC) and high performance concrete. However, the material's damage and fracture mechanisms at meso/micro scales are not well understood, limiting its wider applications considerably. This study aims at an in-depth understanding of the damage and fracture mechanisms of UHPFRC, combining microscale in-situ X-ray computed tomography (µXCT) experiments and mesoscale image-based numerical modelling.

Firstly, in-situ µXCT tests of small-sized UHPFRC specimens under wedge splitting loading were carried out, probably for the first time in the world, using an in-house designed loading rig. With a voxel resolution of 16.9µm, the complicated fracture mechanisms are clearly visualised and characterised using both 2D images and 3D volumes at progressive loading stages, such as initiating of micro-cracks, arresting of cracks by fibres, bending and pulling out of fibres and spalling of mortar at the exit points of inclined fibres.

Secondly, based on the statistics of pores in the µXCT images obtained for a 20mm cube specimen, an efficient two-scale analytical-numerical homogenisation method was developed to predict the effective elastic properties of the UHPFRC. The large number of small pores were first homogenised at microscale with sand and cement paste, using elastic moduli from micro-indentation tests. 3D mesoscale finite element models were built at the second scale by direct conversion of the µXCT images, with fibres and large pores were faithfully represented. The effects of the volume fraction and the orientation of steel fibres on the elastic modulus were investigated, indicating that this method can be used to optimise the material micro-structure.

Thirdly, 3D mesoscale finite element models were built for the specimen used in the in-situ µXCT wedge splitting test, with embedded fibre elements directly converted from
the µXCT images. The fracture behaviour in the mortar was simulated by the damage plasticity model available in ABAQUS. Finally, 2D mesoscale finite element models were developed to simulate the fracture behaviour of UHPFRC using cohesive interface elements to simulate cracks in the mortar, and randomly distributed two-noded 1D fibres and connector elements to simulate the pull-out behaviour of fibres. This approach offers a link between the fibres pull-out behaviour and the response of the whole composite at the macroscale, thus it can be used to conduct parametric studies to optimise the material properties.
Declaration

University of Manchester

PhD by Candidate Declaration

Candidate Name: Ansam Qsymah

Faculty: Engineering and Physical Sciences

Thesis Title: In-situ X-ray computed tomography tests and numerical modelling of Ultra High Performance Fibre Reinforced Concrete

Declaration

I declare that no portion of this work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

--------------------
Ansam Qsymah

Signed:

Date:
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Dedication

This thesis is dedicated to:

Allah, my Creator and my Master;

My great teacher and messenger, Mohammed (May Allah bless and grant him), who taught us the purpose of life;

My great parents, parents-in-law, my dearest husband Jamal Mubarak, my beloved kids: Fares, Mohammad and Amen and my beloved brothers and sisters;

My uncle Dr Mohammad and Memory of my uncle Dr Yousef Qsymah;

All the people in my life who touch my heart;

I dedicate this research.
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Nomenclature

$A$  
Cross-sectional area

$A$  
Stress localisation tensor or concentration tensor

$a$  
Anisotropy ratio

$C_{ijkl}$ or $C_{ij}$ or $C$  
Elastic stiffness tensor

$C_{ij}^H$  
Homogenised elastic stiffness matrix

$d$  
Damage index

$d_t$  
Damage index in tension

$d_c$  
Damage index in compression

$d_f$  
Fibre diameter

$d_e$  
Equivalent diameter of pores

$E$  
Elastic modulus

$E_H$  
Homogenised elastic modulus

$F$  
Applied load

$f$  
Volume fraction

$f'$  
Snubbing coefficient

$G$  
Shear modulus

$G_H$  
Homogenised shear modulus

$G_f$  
Fracture energy

$I, I_{ijkl}$  
Unit tensor

$k_{n0}$  
Normal cohesive elastic stiffness

$k_{t0}$  
Shear cohesive elastic stiffness

$k$  
Bulk modulus

$k_H$  
Homogenised bulk modulus

$l$  
RVE side length

$l_c$  
Critical fibre length

$l_e$  
Fibre embedment length

$l_f$  
Fibre length

$N_f$  
Number of fibres
\( n_i \)  
Unit vector at \( x_i \)

\( P_p^0 \)  
Eshelby's tensor

\( P \)  
Pull-out load

\( S_{ijkl} \) or \( S_{ij} \) or \( S \)  
Compliance matrix

\( s \)  
Boundaries of a volume element

\( t_n \)  
Normal cohesive traction

\( t_s \)  
Shear cohesive traction

\( t_i \)  
Traction in the direction \( i \)

\( u_i \)  
Displacement in the direction \( i \)

\( V \)  
Volume

\( \dot{v} \)  
Periodic fluctuation

\( x_i \)  
Position, \( i=1, 2, 3 \) corresponding to global axes: \( x, y \) and \( z \).

\( W_p \)  
Fibre pull-out energy

\( w_t \)  
Crack open mouth displacement

\( z \)  
Length of debonded zone

\( \Delta \)  
Fibre end slip

\( \alpha_f \)  
Constant to relate the pull-out force from plain concrete to the pull-out force from a composite

\( \beta \)  
Constant to determine the effect of fibre orientation on the slip

\( \gamma \)  
Experimental constant used to determine \( \beta \)

\( \delta \)  
Cohesive separation

\( \delta_{m} \)  
Effective relative displacement

\( \delta_{ij} \)  
Kronecher delta

\( \varepsilon, \varepsilon_{ij} \)  
Strain tensor

\( \varepsilon_c \)  
Compressive strain

\( \varepsilon_t \)  
Tensile strain

\( \zeta \)  
Constant for determining the initial slope of the frictional slip

\( \eta_i \)  
Orientation factor

\( \theta \)  
In-plane angle a fibre

\( \kappa \)  
Fibre-matrix bond modulus
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<td>$\mu$</td>
<td>Friction coefficient</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
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<td>$\nu_H$</td>
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<td>$\tau_f$</td>
<td>Frictional bond shear stress</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Wedge angle</td>
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<tr>
<td>$\phi$</td>
<td>Out-of-plane angle a fibre</td>
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<tr>
<td>$\omega$</td>
<td>Spalling coefficient</td>
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### Acronyms and Terminology

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AE</td>
<td>Acoustic emission</td>
</tr>
<tr>
<td>CCM</td>
<td>Cohesive crack model</td>
</tr>
<tr>
<td>CDPM</td>
<td>Concrete damage plasticity model</td>
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<tr>
<td>CIE</td>
<td>Cohesive interface element</td>
</tr>
<tr>
<td>μXCT</td>
<td>Microscale X-ray computed tomography</td>
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<tr>
<td>DCM</td>
<td>Discrete crack model</td>
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<tr>
<td>FE</td>
<td>Finite element</td>
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<tr>
<td>EHP</td>
<td>Effective homogenised properties</td>
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<tr>
<td>FPZ</td>
<td>Fracture process zone</td>
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<tr>
<td>FRC</td>
<td>Fibre reinforced concrete</td>
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<tr>
<td>GGBS</td>
<td>Ground granulated blast-furnace slag</td>
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<tr>
<td>IBM</td>
<td>Image-based modelling</td>
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<td>ITZ</td>
<td>Interfacial transition zone</td>
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<td>MT</td>
<td>Mori-Tanaka</td>
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<td>KUBC</td>
<td>Kinematic uniform boundary conditions</td>
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<td>PBC</td>
<td>Periodic boundary condition</td>
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<td>RVE</td>
<td>Representative volume element</td>
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<td>SCM</td>
<td>Smeared crack model</td>
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<td>SUBC</td>
<td>Static uniform boundary conditions</td>
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<tr>
<td>UHPFRC</td>
<td>Ultra high performance fibre reinforced concrete</td>
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<tr>
<td>UPV</td>
<td>Ultrasonic Pulse Velocity</td>
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Chapter 1: Introduction

1.1 Motivation
Fibres are often added to a cementitious material to increase its strength, ductility and toughness (Shah & Ouyang, 1991; Li et al., 1991; Naaman, 2007). Different types of fibre reinforced concrete (FRC) are now used widely in structural members such as slabs, beams and walls. Investigating the properties and behaviour of FRC by physical experiments and numerical modelling aids the development of new classes of FRC. For example, Li (2003) has developed a new class of FRC, called engineered cementitious composite, by tailoring the micro-structure of the composite to produce desirable macroscopic properties. This composite has fracture resistance up to 500 times that of conventional concrete but weighs only 60% of the latter. Also, it has ductility of at least two orders of magnitude higher than normal concrete. However, the relatively high material and manufacturing costs and the lack of design codes for some types of FRC still limit their wide acceptance in construction engineering, in spite of a great deal of research being conducted.

One of the most promising cement-based fibre reinforced composite with superior properties and great potentials is Ultra High Performance Fibre Reinforced Concrete (UHPFRC). UHPFRC has been increasingly used in structures such as airport and highway pavements, earthquake and impact resistant structures, tunnels, bridges, hydraulic structures, etc. It is also applied widely for the retrofitting of existing structures (Shah & Ribakov, 2011). As a result of increased applications, extensive experiments have been carried out to obtain the mechanical properties of UHPFRC, and develop proper design methods. However, experiments are often extensive, difficult and costly to carry out, especially if the effects of the phase distributions, volume fractions and local micro-structures are investigated.

In recent years, there has been increasing demand for developing mesoscopic models for cement-based fibre reinforced composites considering the random meso-structure of the material. Failure mechanisms of FRC are intrinsically intertwined with non-homogeneity and randomness at small scales due to the random distribution of fibres and pores. Homogeneous material-based numerical models, using mean field data for heterogeneous
materials, can predict unrealistic smooth crack trajectories and possibly unreliable load-carrying capacity (Yang, Su, et al., 2009). Mesoscale models lead to better understanding of the relationship between the material's meso-structure and the resultant mechanical properties at the macro-level. Moreover, modelling fibres explicitly allows the investigation of the impact of their distribution and orientations on the mechanical properties of FRC (Bolander et al., 2008).

Recently, microscale X-ray computed tomography (μXCT), the 3D imaging technique routinely used in hospitals, has become popular in studying the behaviour of different materials and characterising their internal nano, micro and mesoscale structure (Maire & Withers, 2014; Stock, 1999). This is mainly because of its high resolution, non-destructive nature, and clear visualisation of shapes, sizes and distribution of multi-phases, including pores and cracks. This technique allows the characterisation of the evolution of material behaviour through recording several scans at different time intervals under changing conditions. Applying this technique to in-situ tests of UHPFRC specimens will lead to a better understanding of the process of crack development in this material, and will offer a solid foundation for developing accurate theoretical and numerical models. In-situ μXCT tests of UHPFRC, however, has not been reported to the best knowledge of the author.

As the detailed literature review in Chapter 2 reveals, there is also a pressing need for robust and accurate numerical models for UHPFRC that can link the material micro-/meso-structures and its mechanical properties at macroscale.

1.2 Aims and objectives

This study aims at a deep understanding of the mechanical behaviour of UHPFRC, by combining the μXCT technique and mesoscale numerical modelling. The μXCT is used to characterise the internal micro-structure and the damage evolution process in UHPFRC specimens. The obtained μXCT images are employed to build image-based finite element (FE) models that faithfully represent the internal structure. The specific objectives are:

(1) to design and conduct in-situ μXCT wedge splitting tests of UHPFRC specimens and to characterise and visualise the damage evolution. The cracking patterns and the
toughening mechanisms will be characterised and analysed at different loading stages using the µXCT images;

(2) to statistically analyse the internal micro-structure of UHPFRC specimens, including the volume fraction of phases, initial defects (pores) and overall fibre orientation, using the µXCT images;

(3) to build 3D finite element models for the in-situ wedge splitting test with actual fibre distribution and orientation based on the µXCT images;

(4) to build a 2D finite element model at mesoscopic scale, using a discrete crack approach. This model will be used to conduct parametric studies to investigate the effects of the orientation, length and volume fractions of fibres, on the overall behaviour of the UHPFRC;

(5) to develop an efficient and accurate µXCT image-based multiscale homogenisation method to predict effective elastic properties of the UHPFRC. Analytical and numerical homogenisation methods will be explored. The method will be then used to study the effects of fibre content and fibre orientation on the elastic properties of the UHPFRC. The constituents' properties will be obtained by micro-indentation tests.

1.3 Outline of the thesis

This PhD thesis consists of seven chapters as follows:

Chapter 1 presents the research motivation followed by the research aim and objectives and the outline of the thesis.

Chapter 2 provides a literature review on the UHPFRC and the existing models, focusing on the multiscale and mesoscale models. Introduction to numerical fracture models, image-based modelling, homogenisation methods and principles of the µXCT technique are also presented.

Chapter 3 presents 2D mesoscale finite element models for the tensile behaviour of UHPFRC, using cohesive interfacial elements and discrete fibres representation. This model is then used to conduct parametric studies to investigate the impact of some fibres'
parameters on the UHPFRC tensile response, including the content, length and orientation of fibres.

Chapter 4 presents in-situ μXCT wedge splitting tests conducted on notched UHPFRC specimens. The in-situ test procedures, image processing and segmentation, characterisation of the specimen's internal micro-structure, observations of the evolution of the matrix cracking as well as the damage mechanisms shown in the μXCT images are described and analysed in detail.

Chapter 5 presents the development of a 3D μXCT image-based multiscale homogenisation method for the prediction of effective elastic properties of UHPFRC, combining both analytical and numerical homogenisation approaches. The effects of fibre content and orientation on the elastic properties of the UHPFRC are investigated.

Chapter 6 presents the development of finite element models to simulate the fracture behaviour of the μXCT wedge splitting test presented in Chapter 4. The results are compared with the experimental data.

Chapter 7 draws the main conclusions with suggestions for future research.
Chapter 2: Literature Review

In this chapter, an introduction to the UHPFRC and the pull-out behaviour of short fibres, numerical modelling of fracture in cementitious composites, image-based modelling and homogenisation methods, will be presented. The existing numerical models, with an emphasis on the mesoscale and multiscale models, will be reviewed. A review of non-destructive techniques, specifically the µXCT and its application in the material studies, will be also conducted.

2.1 The material and basic mechanical properties

UHPFRC is characterised by high compressive strength, tensile strength and ductility. For example, Wille et al. (2012) have achieved compressive strength up to 292MPa, tensile strength up to 37MPa, and strain at the peak stress of 1.1% at 28 days by using 8% by volume of high strength steel fibre. This material is also characterised by a very high fracture energy of up to 40,000 J/m$^2$ (Millard et al., 2010) and excellent impact and blast resistance (Li et al., 2015; Mao et al., 2014). These properties are achieved by using a high cement content, low water to binder ratio (<0.2), fine sand (average size <0.5mm), microsilica or silica fume, and a sufficient amount of superplasticiser (Le, 2008; Yang, Millard, et al., 2009; Wille et al., 2012). To ensure proper fibre package coarse aggregates are not used (Richard & Cheyrezy, 1995). Different types of fibres can be used such as glass, carbon, polymer and steel fibres with different shapes and aspect ratios. To improve bonding with the surrounding matrix, fibres can be subjected to chemical and physical surface treatments such as degreasing, surface roughness and surface coating (Shah & Ouyang, 1991).

Generally, it has been suggested that concrete with a compressive strength over 150MPa can be described as Ultra High Performance Concrete (UHPC), and when fibres are added the term UHPFRC is used (Wille et al., 2012). In this thesis, the term UHPFRC is used. Other terms such as Reactive Powder Concrete (RPC) and strain-hardening cementitious composites (SHCC) have also been used in the literature to describe this material (Kunieda et al., 2011; Naaman, 2007; Richard & Cheyrezy, 1995).
The post cracking behaviour of the UHPFRC under tensile loading is quite different than that for conventional FRC. As seen in Figure 2.1, the conventional FRC exhibits strain-softening behaviour after the first cracking accompanied by immediate localisation of deformation in a single crack, while UHPFRC shows a strain hardening response accompanied by multiple cracking with ultimate tensile strength $\sigma_{pc}$ higher than the first cracking strength $\sigma_{cc}$ (Naaman, 2007; Li, 1992). The strain-hardening behaviour is a very desirable property because it increases the strain capacity of the composite (Naaman, 2007). An even distribution of fibres and a strong bond between the fibres and the surrounding matrix is essential to achieve this behaviour (Hassan et al., 2012).

Figure 2.1 Typical stress-strain curves in tension for conventional FRC and UHPFRC (Naaman, 2007).
The tensile stress-strain curve of UHPFRC can be divided into three distinct stages as seen in Figure 2.1: the linear elastic stage up to 90-95% of the cracking strength \( \sigma_{cc} \) (Hassan et al., 2012; Wille et al., 2011), the strain hardening stage accompanied by the development of multiple micro-cracks distributed along the specimen and strain softening stage at which the width of one or more cracks increases to form macro-cracks, while the fibres bridging them are subjected to pull out. Strain is no longer evenly distributed in the latter stage, thus the softening behaviour is expressed as a function of the opening of the mouth of the localised crack. The maximum crack width is assumed to be equal to half of the fibre length (Li et al., 1991; Naaman, 2007).

The post cracking behaviour of UHPFRC is quite important to achieve the successful application of this material (Bentur et al., 1985; Shah & Ouyang, 1991). If most of the fibres rupture under loading, the composite will not show tension softening behaviour. Therefore, fibre rupture should be prevented by tailoring the interfacial zone between the fibres and the surrounding matrix to force most of the fibres to experience pull-out behaviour.

### 2.2 Fibre pull-out behaviour

The main role of fibres is to bridge cracks developed in the cementitious matrix and transfer stress across the crack faces through the bond between the fibres and the surrounding matrix (Lin & Li, 1997). The bond between the fibre and the matrix is characterised as the weakest zone in the FRC (Li, 1992; Shah & Ouyang, 1991). The bridging fibres are subjected to pull-out forces which lead to fibre debonding and slip, as seen in Figure 2.2. The debonding process can be described as a tunnel crack that propagates along the fibre-matrix interface from the matrix crack surface toward the embedded end (Figure 2.2a). The debonded part of the fibre stretches, while its deformation is constrained by the friction at the fibre-matrix interface. After complete debonding, the fibre slip out of the matrix (Figure 2.2b). The slip of fibre is resisted by the friction at the fibre-matrix interface (Figure 2.2c) (Naaman & Najm, 1991; Naaman et al., 1991a, 1991b). Debonding and pull-out are of great importance in toughening the cementitious matrix (Li, 1992; Trainor et al., 2012). However, for hooked end fibres and deformed fibres, the pull-out resistance is primarily controlled by the mechanical bond.
between the fibre deformations and the surrounding concrete (Banthia & Trottier, 1994). The hooked end fibres and the deformed fibres are not considered in the present study.

![Diagram of fibre pull-out tests](image)

Figure 2.2 Debonding and pull-out of a smooth straight fibre from a matrix (Cunha, 2010).

For accurate predictions of UHPFRC properties, it is necessary to characterise the interface behaviour under loading. Pull-out tests have been frequently conducted to assess the mechanical properties of the fibre-matrix interface (Banthia & Trottier, 1994; Cunha, 2010; Lee et al., 2010; Naaman & Najm, 1991). There are different configurations for the pull-out tests; the simplest one is single fibre embedded at one of its ends and the load is applied on its free end as shown in Figure 2.2. In these tests, the fibre-matrix interface behaviour is characterised by determining the relationship between the applied load ($P$) and the fibre slip ($\Delta$). In spite of the belief sometimes held that there is no correlation between the behaviour of a fibre in pull-out tests and its behaviour in a real structure (Maage, 1977), the data obtained from these tests is commonly used to characterise the bond between fibres and the surrounding matrix and to optimise the material properties (Banthia & Trottier, 1994).

The maximum pull-out load ($P_{\text{max}}$) measured during the pull-out test is used to calculate the average bond strength ($\tau_{\text{max}}$) between a fibre and the surrounding matrix using the following expression:

$$\tau_{\text{max}} = \frac{P_{\text{max}}}{\pi d_f l_e}$$ (2.1)

where $d_f$ is the fibre diameter and $l_e$ is the initial embedded length of the fibre. The post-cracking strength is directly related to the average bond strength $\tau_{\text{max}}$ of the fibre-matrix
interface (Li et al., 1991). Moreover, the fibre pull-out energy \( W_p \), which is defined as the area under \( P - \Delta \) curve, can be calculated using:

\[
W_p = \int_{\Delta=0}^{\Delta=\Delta_e} P(\Delta)d\Delta
\]  

(2.2)

Equation 2.1 shows that \( \tau_{\text{max}} \), usually assumed as a material property for the interfacial zone, depends on the fibre dimensions. To develop a more realistic model that describes this material property, stress distributions in the fibre and in the surrounding matrix need to be known. Several fibre pull-out models have been proposed to find the stress distributions, and then estimate the constitutive relationship of the fibre-matrix interface. They can be classified according to the debonding criterion through two different approaches: the fracture mechanical approach and the stress approach (Gray, 1984; Shah & Ouyang, 1991; Stang et al., 1990). When the debonding criterion is satisfied, the debonded zone propagates. The fracture-based models assume that the propagation of debonding zone requires an adequate energy at the interface material to drive the debonding process forward (Lin et al., 1999; Zhang & Li, 2002). In the stress-based approach, the debonded zone is assumed to advance once the shear stress at the bonded zone reaches the shear strength of the interface. The continuation of the debonding is governed by the interfacial friction stress which is independent of the fibre diameter (Gopalaratnam & Shah, 1987; Lawrence, 1972; Leung & Li, 1991; Nammur & Naaman, 1989). The debonding criterion is a material characteristic and depends on the fibre and matrix type (Li & Chan, 1994).

The pull-out behaviour of steel fibre depends on many parameters such as: matrix composition and strength; fibre type and geometry; fibre embedment length; fibre orientation; fibre diameter and the environmental conditions (Cunha, 2010).

### 2.2.1 Effect of fibre orientation angle

In random fibre composites, most of the fibres lie at an angle to the crack plane. The orientation angle between fibres and the crack plane has a significant effect on pull-out behaviour. Besides fibre debonding and pull-out, inclined fibres exhibit more damage mechanisms than fibre oriented perpendicularly to the crack surface. These mechanisms
include fibre bending and spalling of the matrix at the fibre exit point (Leung & Chi, 1995; Li, 1992; Ouyang et al., 1994).

When an inclined fibre bridges a crack, geometric restrictions cause fibre bending (Figure 2.3). The pull-out load of an inclined fibre \( P_\phi \) can be decomposed into two components: a debonding (and pull-out) component along the fibre axis \( P_x \) and a bending component perpendicular to the fibre axis \( P_y \). The pull-out load in the inclined fibre increases due to the frictional concentration at the point at which the fibre exits the matrix, leading to an increase in the efficiency of the fibre in resisting the crack growth (Ouyang et al., 1994; Cunha, 2010; Lee et al., 2010).

![Figure 2.3 Bending of an inclined fibre bridge a crack and matrix spalling below the fibre (shaded area) (Leung and Chi, 1995).](image)

The increase in the value of the pull-out load due to fibre inclination can be accounted for using the empirical relation (Li, 1992; Li et al., 1990):

\[
P(\phi) = P(\phi = 0)e^{\ell\phi}
\]  

(2.3)
where $P(\phi)$ is the pull-out load of the inclined fibre; $\phi$ is the orientation angle in radians; $P(\phi = 0)$ is the pull-out load of the fibre that is perpendicular to the crack plane and $\hat{f}$ is the snubbing coefficient and its value can be determined experimentally. This empirical equation has been widely used in the literature for synthetic and steel fibres due to its simplicity. The value of $\hat{f}$ varies according to the type of fibre and the matrix. Its value ranges between 0.5 and 1 for nylon and polypropylene fibres embedded in a normal strength mortar (Kunieda et al., 2011; Li, 1992; Lin et al., 1999). Schauffert & Cusatis (2011) adopted a lower value ($\hat{f}=0.4$) for conventional steel fibre reinforced concrete. For UHPFRC, Lee et al., (2010) reported a value of 1.6.

Also, the supporting matrix experiences local spalling in the region where the inclined fibre exits the matrix due to stress concentration induced by the fibre bending. The length of the spalled matrix is governed by the fibre bridging force, matrix strength and fibre inclination angle (Leung & Chi, 1995; Leung & Li, 1992). The spalling mechanism reduces the embedded length of the fibre by the spalling length, and as a result, the pull-out force decreases and the corresponding crack opening displacement increases.

2.2.2 Effect of fibre length
Increasing the length of the fibre increases the contact area between the fibre and the surrounding matrix; and thus a higher frictional resistance is obtained at the fibre-matrix interface. A long embedment length enables the fibre to sustain higher bridging forces, and as a result, fibre stresses could reach the fibre strength, leading to fibre rupture and poor post peak behaviour (Li, 1992; Shannag et al., 1997). The optimal fibre length for aligned fibre can be estimated using the concept of critical embedment length ($l_c$) given by (Li, 1992; Li et al., 1991):

$$l_c = \frac{d_f \sigma_f^u}{4\tau_{max}}$$  \hspace{1cm} (2.4)

where $\sigma_f^u$ is the fibre rupture strength. To ensure that all fibres in the composite experience a pull-out response with the maximum amount of frictional work without rupturing, the optimal fibre length should be close to the critical length but no more than $2l_c$ (Li et al., 1991).
2.2.3 Effect of matrix strength
The pull-out performance has been shown to be enhanced by using high strength matrix (Abu-Lebdeh et al., 2011; Chan & Chu, 2004; Shannag et al., 1997). The peak pull-out load as well as the pull-out energy increase with the increasing compressive strength of the matrix. Shannag et al. (1997) found that the peak pull-out load of a straight steel fibre is almost doubled when the compressive strength of the mortar matrix is increased from 40 to 150MPa. Moreover, the frictional decay following the peak load is eliminated for the higher matrix strength, and the pull-out work is much larger.

These improvements in the pull-out resistance are attributed to the enhanced interfacial micro-structure in high strength fibre reinforced concrete. In cementitious composites, a weak interfacial transition zone (ITZ) is usually formed between the matrix and the embedded inclusions (fibres or sand), that has a strength less than the bulk matrix. The bond between the matrix and the fibres depends on the properties of this weak zone rather than on the bulk matrix. In conventional FRC, this layer could be 50~100µm thick (Shah & Ouyang, 1991). However, in UHPFRC the mortar matrix is highly densified by eliminating the coarse aggregate, using a lower water to binder ratio and mineral admixtures. As a result, the thickness of the interfacial zone is reduced to about 1~5µm (Damidot et al., 2003).

2.3 Fracture modelling
Cement-based materials are basically quasi-brittle materials with strain softening behaviour after peak load. This behaviour is attributed to the existence of a fracture process zone (FPZ) in front of the macroscopic crack. Figure 2.4 shows the FPZ formed in FRC due to the fibre bridging mechanism and micro-cracking. The nonlinear behaviour of the FPZ in cement-based materials is modelled by one of the following popular approaches: Smeared Crack Model (SCM) (proposed by Bažant & Oh, 1983) and Discrete Crack Model (DCM) (proposed by Hillerborg et al., 1976). These approaches model the FPZ in different ways, while the bulk material is assumed as elastic. Many researchers have proposed comparative studies between these two approaches (De Borst, 2003; Jendele et al., 2001; Rots, 1991). So far, there is no consensus in the literature which model is better for modelling cementitious composites.
In SCM, the FPZ is represented as a continuum in which many micro-cracks are uniformly distributed (smeared) perpendicular to the principal stress direction over certain width. The constitutive relationship (expressed as stress versus strain) is modified in the vicinity of the crack to capture the deterioration of the FPZ. SCM offers a variety of approaches according to the cracking direction, including a fixed single crack model and a rotating crack model. In the fixed crack model, the crack orientation is kept constant during the entire computational process, while the rotating crack model allows the crack to rotate continuously with the axis of the principal stress (Rots, 1991). SCM can be easily programmed, thus it has been incorporated in a number of finite element codes such as ABAQUS (Simulia, Providence, RI) and DIANA (TNO, Delft, The Netherlands). It can also be generalized to consider the tri-axial stress in the FPZ (Bazant, 2002).

Nevertheless, SCM suffers from several drawbacks. As the dimensions of the finite elements tend to zero, SCM leads to the phenomenon of strain localisation, resulting in the mesh non-objectivity problem. To overcome this disadvantage, various localisation limiters have been developed such as: gradient-dependent models (Schreyer & Chen, 1986), the micro-polar continuum (Mühlhaus & Vardoulakis, 1987) and the non-local continuum model (Jirásek & Bazant, 1994).

Figure 2.4 Fracture process zone in fibre reinforced concrete (Shen et al., 2010).
In DCM, the FPZ is modelled as a fictitious crack as opposed to real cracks with no stress transfer. This fictitious crack is still able to transfer stress (called cohesive stress), which increases from zero at the tip of the stress-free crack to the tensile strength of the material at the tip of the fictitious crack. DCM based on Cohesive Crack Model (CCM), where cohesive interface elements are inserted into existing elemental edges, is now accepted as the simplest and most accurate nonlinear fracture model for cementitious materials (Bazant, 2002; Shi, 2009). The CCM is increasingly used to predict crack propagation in different quasi-brittle materials. This model and its applications were comprehensively reviewed by Chandra et al. (2002).

Nevertheless, DCM suffers from several problems. The finite element implementation using the DCM requires re-meshing to model the curvilinear crack propagation because its location is unknown a priori (Yang & Chen, 2005). Furthermore, the DCM has limitation in modelling tri-axial stress problems and tortuous cracking (Bazant, 2002). However, DCM can give cracking details such as the crack path, spacing and widths (Yang & Chen, 2005). To avoid re-meshing, cohesive interfacial elements can be pre-inserted a priori along the known crack path (Sato et al., 2004), or along all solid element interfaces when the crack path is unknown (Su et al., 2010; Yang, Su, et al., 2009). These nonlinear interface elements increase the computational cost considerably.

2.4 Homogenisation methods

Basically, homogenisation is the process of determining the effective properties of a heterogeneous material (Kanit et al., 2003; Sharma et al., 2013; Zohdi & Wriggers, 2008). Homogenisation methods are widely used to predict the mechanical properties of different types of composites. In this section a brief review on both computational and analytical homogenisation methods are presented.

2.4.1 Computational homogenisation

Computational homogenisation method, mostly using the finite element method, proves powerful in modelling complicated heterogeneous material structures. In this approach, the effective properties of a heterogeneous material can be obtained by averaging the macroscopic properties over a representative volume element (RVE). The homogenised elastic properties of the material can then be evaluated by the linear relationship between
the volume average stress and the volume average strain, using the generalized Hook's law which can be written in terms of homogenised stiffness tensor as:

\[
\langle \sigma_{ij} \rangle = C_{ij}^H \langle \varepsilon_{ij} \rangle \tag{2.5}
\]

where \(\sigma_{ij}\) is the second-order symmetric Cauchy stress tensor, \(\varepsilon_{ij}\) is the second-order symmetric strain tensor, \(C_{ij}^H\) is the homogenised stiffness tensor and the brackets \(\langle \rangle\) are added to indicate the average values for the stress \(\sigma_{ij}\) and the strain \(\varepsilon_{ij}\).

To obtain the components of the stiffness tensor, six independent loading cases were prescribed on the boundaries of RVE to produce a uniform strain (stress) in the RVE. Each loading case consists of surface displacements (or tractions) that render null all but one of the six components of the strain tensor.

The generalized Hook's law can be also expressed in terms of the compliance tensor \(S_{ij}\), which is the inverse of the stiffness tensor \(C_{ij}\), as follows:

\[
\langle \varepsilon_{ij} \rangle = S_{ij}^H \langle \sigma_{ij} \rangle \tag{2.6}
\]

In terms of engineering constants, the compliance matrix components \(S_{ij}\), for an orthotropic material, are (Jones, 1998):

\[
S_{ij} = \begin{pmatrix}
\frac{1}{E_1} & -\frac{v_{12}}{E_1} & -\frac{v_{13}}{E_1} & 0 & 0 & 0 \\
-\frac{v_{21}}{E_2} & \frac{1}{E_2} & -\frac{v_{23}}{E_2} & 0 & 0 & 0 \\
-\frac{v_{31}}{E_3} & -\frac{v_{32}}{E_3} & \frac{1}{E_3} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{G_{23}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_{31}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{G_{12}}
\end{pmatrix}
\tag{2.7}
\]

where \(E_1, E_2\) and \(E_3\) are the Young's moduli in the 1, 2 and 3 directions, and \(G_{23}, G_{31}\) and \(G_{12}\) are the shear moduli in the 2-3, 3-1, and 1-2 planes respectively. \(v_{ij}\) is the Possion's ratio for strain in the \(j\)-direction when stress is in the \(i\)-direction.
If there are an infinite number of planes of material property symmetry, the number of independent elastic constants is reduced to two, resulting in isotropic material in which:

\[ E_1 = E_2 = E_3 = E \]
\[ G_{12} = G_{31} = G_{23} = G \]  
\[ \nu_{12} = \nu_{31} = \nu_{23} = \nu \]

where \( G \) can be expressed in terms of \( E \) and \( \nu \) as follows:

\[ G = \frac{E}{2(1 + \nu)} \]  

(2.9)

2.4.1.1 RVE concept

The common approach to predict the effective properties of a composite material is to define first a statistically representative volume element (RVE) that captures the major features of the composite micro-structure. The classical definition for the RVE is attributed to Hill, (1963), who defined RVE as a volume of the heterogeneous structure that is sufficiently large to be statistically representative of the composite, and at the same time, small enough to be considered as a volume element. This definition implies that a large RVE should be used to ensure that it contains a sufficient number of composite inclusions (particles, fibres, pores, etc.). In the case of composites reinforced with random inclusions, Kanit et al. (2003) has found that the effective elastic properties of these materials can be determined as mean values of the apparent properties of small volumes rather than a large RVE, providing that a sufficient number of RVEs is used. They reported that the size of the RVE depends on five parameters: the physical property, the contrast of properties, the volume fraction of components, the required accuracy and the number of volume elements.

2.4.1.2 Boundary conditions

Different boundary conditions can be imposed on the RVE. As a matter of fact, the response of the RVE must not change with the type of the imposed boundary conditions. However, this could require a large size of RVE (Kanit et al., 2003). Generally, there are three types of boundary conditions that are used in connection with the RVE concept (Kanit et al., 2003):
(1) Kinematic uniform boundary conditions (KUBC): the displacement $u_i$ is imposed at point $x_i$ belonging to the boundary $s$:

$$u_i(s) = \varepsilon_{ij}x_i, \quad \forall \ x \in s$$  \hspace{1cm} (2.10)

(2) Static uniform boundary conditions (SUBC): the uniform traction vector $t_i$ is prescribed at the boundary $s$:

$$t_i(s) = \sigma_{ij}n_i, \quad \forall \ x \in s$$  \hspace{1cm} (2.11)

where $\varepsilon_{ij}$ and $\sigma_{ij}$ are symmetrical second-rank tensors of the components of the applied strain and stress respectively that do not depend on $x_i$, and $n_i$ is a vector normal to the boundary $s$ at point $x_i$.

(3) Periodic boundary conditions (PBC): the periodic displacement field $u_i$ is imposed at point $x_i$ belonging to the boundary $s$:

$$u_i(s) = \varepsilon_{ij}x_i + \hat{v}, \quad \forall \ x \in s$$  \hspace{1cm} (2.12)

where $\hat{v}$ is the periodic fluctuation field and it takes the same values on opposite faces of the RVE (Kanit et al., 2003).

When using volumes smaller than the RVE, the obtained properties are described as the "apparent" properties of the material. Increasing the size of the volume, the apparent properties converge towards the "effective" properties. It has been shown that the "effective" properties of a composite material can be obtained from a relatively smaller RVEs by using PBC, rather than KUBC or SUBC (Kanit et al., 2003).

**2.4.3 Analytical homogenisation**

The classical analytical homogenisation methods are considered as an alternative for the computational homogenisation techniques. The simplest method to estimate the effective elastic modulus of a composite analytically is by using the conventional upper and lower bound solutions, or a combination of the two. The estimation is usually based on the volume fractions ($f$) and elastic moduli ($E$) of both matrix and the embedded inclusion. The widely used upper- and lower- bound solutions are Voigt's and Ruess's bounds (Hill,
1963), which are obtained by neglecting any particular morphological arrangements of the phases. Hashin and Shtrikman, (1963) proposed a variational principle for finding upper and lower bounds of average elastic moduli of composite materials. These bounds are used widely for materials with high contrast of the properties of the constituents.

One of the most notable analytical homogenisation model is the Eshelby's equivalent approach (Eshelby, 1957), which is based on an ellipsoidal inclusion in an elastic infinite matrix. According to this model, the microscopic strain within the inclusion $\varepsilon_p$ is linked with the applied strain at the boundary $\varepsilon$ through:

$$\varepsilon_p = \left[ I + P^0_p : (C_p - C_0) \right]^{-1} : \varepsilon$$

where $I$, $I_{ijkl} = 1/2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj})$, is the fourth-order unity tensor, $\delta_{ik}$ is the Kronecker delta, $C_p$ is the stiffness of the inclusion, and $C_0$ is the stiffness of the matrix. The fourth-order tensor $P^0_p$, is called Eshelby tensor. The Eshelby model served as a basis for many other models that based on mean field inclusion approach such as Mori-Tanaka (MT) scheme (Benveniste, 1987; Mori & Tanaka, 1973), the self-consistent approach (Hill, 1965), and generalized self-consistent scheme (Christensen & Lo, 1979). Among these models, the MT scheme is of particular interest.

The applicability of the MT scheme on cement-based materials has been justified by many researchers (Bary et al., 2009; Constantinides & Ulm, 2004; Da Silva et al., 2014; Ghabezloo, 2010; Sorelli et al., 2008). It was shown by Bary et al. (2009) that the MT scheme gives relatively more accurate estimations of the elastic moduli of cementitious materials than other approaches. Its simplicity makes it even more attractive.

In MT scheme, each inclusion is considered as an inclusion embedded in an infinite matrix and is subjected to a "fictitious" displacement boundary condition. The applied strain $\varepsilon$ is set equal to the volume average strain over the RVE with multiple inclusions $\langle \varepsilon_{ij} \rangle_{RVE}$:

$$\langle \varepsilon_{ij} \rangle_{RVE} = \varepsilon$$

The single particle problem is solved first based on Eshelby's solution of an ellipsoidal inclusion subjected to a fictitious uniform strain boundary condition of the form:
\[ u = \epsilon_0 \cdot x \] (2.15)

where \( \epsilon_0 \) is the macroscopic strain for the single particle RVE. The strain in the inclusion \( \epsilon_p \) is related to \( \epsilon_0 \) by strain localisation tensor \( A \) as follows:

\[ \epsilon_p = A : \epsilon_0 \] (2.16)

where \( A \) is function of the Eshelby tensor, the local elasticities and the volume fraction of the phases. Equations 2.14 and 2.16 imply that:

\[ \epsilon = (A)_{RVE} : \epsilon_0 = (A)^{-1}_{RVE} : \epsilon \] (2.17)

Substituting equation 2.17 into 2.16 yields the inclusion strain in the form:

\[ \epsilon_p = (A)_{MT} : \epsilon; A_{MT} = A : (A)^{-1}_{RVE} \] (2.18)

where \( A_{MT} \) is the localised tensor relating the inclusion strain to the real far field strain \( \epsilon \). The modified localisation tensor \( (A)^{-1}_{RVE} \) allows for interaction between particles to be considered.

### 2.5 Image-based modelling

Image-based modelling (IBM) allows for converting the real internal structure of a material to FE meshes that represent faithfully the size, shape and distribution of each phase (Chen et al., 2004; Smith et al., 2014; Yue et al., 2003). The actual internal structure of a material can be acquired by digital image techniques such as high resolution digital cameras or X-ray scanners, and the images can then be transformed into FE meshes for mechanical analysis. IBM offers a practical approach for designing and optimising materials with complex internal structures for user-specified properties without the need for costly experimental tests.

The acquired images can be transformed into finite element meshes by two different ways (Chen et al., 2004): voxel-based meshing approach and surface-based meshing approach. In the first approach, each voxel/pixel in the image is directly converted into a same-sized finite element, allowing for accurate modelling of complex morphologies of multiphase materials. Despite the simplicity of this approach, it is very computationally expensive because of using a large number of finite elements equal to the number of voxels/pixels in the image. Alternatively, the meshes can be generated using a surface-based approach, in
which the mesh size is reduced and optimised by sophisticated mesh generation algorithms (Chen et al., 2004; Yue et al., 2003). Nevertheless, this approach could involve significant manual operations to simplify the geometric mesh, resulting in loss of accuracy (Antiga et al., 2002; Huang et al., 2015).

The recent development of imaging techniques and their applications on wide range of materials raises the demand for efficient ways of image transformation. Commercial software packages such as AVIZO (VSG, Burlington, MA) and ScanIP (Simpleware Ltd, UK) can be used to segment images into distinct regions to locate objects and boundaries, and then convert them into FE meshes. However, these processes require significant user interaction and simplifications to obtain the desired meshes. The requirement for more advanced computer programs is still an open issue for more accurate image-based models (Huang et al., 2015).

2.6 Modelling of FRC

The existing models of FRC can be classified according to the scale of observation into: micro-, meso- and macro-models (Figure 2.5). Models at small scale (micro- and meso-models) consider explicitly the heterogeneity and the randomness of the FRC internal structure (Bolander & Saito, 1997; Cunha et al., 2012; Kang et al., 2014; Li et al., 1991; Lin & Li, 1997; Radtke et al., 2010 and 2011). These models help in linking the local phenomena at small scale (such as fibre-matrix interface constitutive law) and the structural response at the macroscale.

![Figure 2.5 Scales of observation for engineering structures (Van Mier, 1997).](image-url)
At the macroscale, the FRC is modelled as a continuum homogeneous material using the stress-strain relationship of the whole composite as an input in the model (Beghini et al., 2007; Li et al., 1998; Mahmud et al., 2013). This simple approach is desirable for the purpose of structural analysis to investigate the load-bearing capacities of structural members.

It is also possible to combine more than one scale in a single model (multiscale models), in which the results obtained at small scales can be used to predict the behaviour of complex materials or structures at larger scales (Gal & Kryvoruk, 2011; Kabele, 2007; Qsymah et al., 2015; Sorelli et al., 2008). The existing mesoscale and multiscale models are reviewed in detail in the next sections.

2.6.1 Mesoscale models

There has been a trend in recent years towards developing FRC models by representing it as a three-phase material: unreinforced concrete/mortar matrix, fibres, and fibre-matrix interface. These models allow the investigation of the effects of fibre parameters such as: content, orientation and distribution of fibres, on the composite behaviour at the macroscale directly. Limited numerical studies have modelled FRC at mesoscale, due to the presence of a large number of randomly distributed short fibres which results in high computational cost. Moreover, there are difficulties in modelling the interaction of fibres with the surrounding matrix effectively. The existing FRC mesoscale models are mainly based on: discrete models; cohesive crack models and continuum models.

Within the framework of discrete models, several mesoscale models were proposed to simulate the tensile and flexural behaviour of FRC. In this approach, the continuum (representing the matrix) is replaced by a system of discrete elements intended to represent aggregate particles and their interaction (Cusatis et al., 2003). The discrete models were intended first to study concrete fracture, and then extended for FRC by adding the fibre reinforcement. Using this approach several two- and three-dimensional models were proposed in the literature.

Bolander and Saito, (1997) used discrete model approach to simulate the tensile behaviour of FRC in 2D. The pull-out behaviour of the fibres was represented by
nonlinear spring elements that were lumped between adjacent matrix elements and aligned with the fibre direction, so that they connect two cells at the points where fibres cross the common boundary. This model was further developed and refined in subsequent studies such as (Bolander et al., 2004; Bolander et al., 2008). Kunieda et al. (2011) followed the same approach to simulate the tensile behaviour of the UHPFRC at the mesoscale. Kang et al. (2014) proposed another way to model the pull-out behaviour of fibres using the same discrete model, but the pull-out behaviour was represented by using nonlinear springs that were distributed along the whole fibre rather than lumped at the crack surfaces. It was shown that the onset and propagation of cracks in these models are strongly affected by the mesh size (Kunieda et al., 2011). The results of these models depend on the shortest embedment length of each fibre. Finer meshes make fibre spans over several matrix elements and therefore the embedment length of each fibre is reduced. In such a case, the load transfer between fibres and the surrounding matrix cannot be properly represented (Bolander et al., 2008). Discrete models were also exploited to model the effect of the fibres by adding their contribution to the matrix response which was modelled as rigid particles (Schauffert & Cusatis, 2012; Schauffert et al., 2012).

A few models were developed for FRC by treating the concrete/mortar matrix as a homogeneous continuum. Radtke et al. (2010) used this approach to develop a model in which the action of the fibres was represented, rather than the fibres themselves. In this model, reaction forces, which were assumed equal to the fibre pull-out forces, were applied on the matrix mesh at the fibre end points. More recently, Radtke et al. (2011) proposed another model for simulating nonlinear debonding and matrix failure in FRC by adding fibres explicitly and embedding them in a continuum matrix. The displacement discontinuities produced by the fibre slippage were represented by enrichment functions using the partition of unity finite element approach.

Using the smeared crack model, Cunha et al. (2011; 2012) proposed a model for FRC in which fibres were represented as 1D two-noded elements that were bonded perfectly to the matrix mesh, while their pull-out behaviours were simulated indirectly. The experimental pull-out load versus slip relationships were first converted to equivalent
stress-strain relationships, and were then used to model the constitutive behaviour of the fibre elements. Soetens et al. (2012) followed this simple approach to simulate the fracture of FRC beam under flexural loading. Modelling fibres and their pull-out behaviour using this approach is simple and computationally cheap. However, it was proven that classical continuum models depend on the size of finite elements, thus the result of the simulation may not be objective (De Borst, 2003; Jendele et al., 2001).

Using a cohesive crack model, Sue et al. (2011) proposed a mesoscale model to simulate the tensile behaviour of the FRC by pre-inserting zero-thickness cohesive elements in the matrix mesh to represent the potential cracks in the matrix. The fibres were modelled as two-noded 1D elements that were bonded perfectly to the matrix mesh, while their interfaces were modelled indirectly through the constitutive laws of the steel fibres, following the approach proposed by Cunha et al. (2011). Similarly, Tarasovs et al. (2016) used a cohesive crack model with zero-thickness cohesive elements to represent the cracking behaviour of the matrix. However, the fibres and their interfaces were replaced by springs connecting coincident nodes of the cohesive elements. In this model the number of fibres that can be inserted in the mesh is restricted to the number of nodes in the matrix mesh, and as a result, a very fine mesh is required when using a large number of fibres.

### 2.6.2 Multiscale models for homogenisation of elastic properties

In recent years, a few multiscale models have been proposed to simulate the elastic properties of FRC using computational and analytical homogenisation methods. Gal and Kryvoruk, (2011) have developed a two-step homogenisation model to predict the effective elastic properties of FRC. The aggregates and the surrounding interfacial zone were homogenised first using the Garboczi's analytical method (Garboczi & Berryman, 2001), and the homogenised aggregates were then integrated with the concrete/mortar matrix to predict the overall elastic properties of the FRC. Zhang et al. (2015) extended this model by taking the interfacial zone between fibres and the surrounding matrix into account.

Using μXCT images, Qsymah et al. (2015) recently have developed two-step image-based numerical homogenisation models for UHPFRC to predict its effective elastic
properties. In the first step, the mortar matrix with a large number of small pores were homogenised, and in the second the fewer large pores and steel fibres were modelled with the homogenised matrix. This leads to significant reduction in computational costs over one-step approaches modelling of all pores.

Sorelli et al. (2008) used the analytical Mori-Tanaka method (MT) (Benveniste, 1987; Mori & Tanaka, 1973) to develop a multiscale model for HPFRC, to upscale the elastic properties of the material constituents through three different levels of observations. The local elastic properties of the individual constituents of the HPFRC were obtained by nano-indentation tests. In spite of the simplicity of this approach, analytical homogenisation methods do not take into account the shape, size and the random distribution of the inclusions.

2.6.3 Multiscale models for fracture simulations

A few multiscale models have been developed to model the fracture behaviour of FRC. Kabele (2007) proposed a sequential multiscale framework for HPFRC by linking analytical and numerical models to simulate its fracture behaviour. At the microscale, phenomena like matrix crack initiation, fibre-matrix interaction and fibre pull-out, were modelled using several analytical models given in the literature (Li et al., 1991; Li & Wu, 1992; Lin et al., 1999). At the mesoscale, the material was modelled analytically using the model developed by (Li et al., 1991) and numerically using representative volume elements for the material in 2D, and the multiple cracking behaviour of the HPFRC was considered. At the macroscale, the FE model was employed to consider the geometrical details of structural members.

Zhan & Meschke, (2013) proposed a multiscale approach using both analytical and numerical models to model the fracture behaviour of the FRC. At the micro-level, the pull-out behaviour of fibres was investigated using analytical and numerical models. The RVE concept was exploited to simulate the composite behaviour at the mesoscale, in which the bridging forces of fibres were obtained by integrating the individual pull-out response of all fibres crossing a crack. At the macroscale, the embedded crack approach was used to analyse the overall material behaviour.
Oliver et al. (2012) proposed a two-scale formulation for analysing the fracture behaviour of the UHPFRC based on the multifield theory. In this approach the macroscale model was endowed with an internal morphology taking into account properties that come from smaller scales such as fibre pull-out behaviour. Here, the fibre can stretch independently of the matrix strain, and the stretching in both fibre and matrix can be coupled by means of an interface having a specific constitutive response. This meso-structural interaction can be modelled by using a new kinematic independent variable.

From this survey of FRC mesoscale and multiscale models proposed in the literature, it can be seen that there are limited studies that represented fibres explicitly. The material's internal structure used in the numerical models (except (Qsymah et al., 2015)) was generated using statistical algorithms with inclusions of assumed simplified shapes and distribution, and little attention is paid to the effect of pores which exist intrinsically in cementitious composites. This is mainly due to the lack of real 3D internal meso-structure and the high computational cost.

2.7 Non-destructive characterisation techniques

The application of advanced non-destructive testing techniques in composite materials has received an increasing attention because they allow for looking inside a material rather than just examine its surface. This ability is of great importance since it enables engineers to characterise the internal fracture behaviour of materials, which can inform the development and validation of computer models. Moreover, non-destructive techniques can be used to assess the achieved material quality and control its properties during casting and after hardening (Shah & Ribakov, 2011). Several non-destructive testing methods have applied on the FRC such as: the electrical resistivity technique; electrochemical impedance spectroscopy; near-field microwave method; ground penetrating radar; X-ray and gamma-ray radiography; acoustic emission and the ultrasonic pulse velocity method. A comprehensive review of the application of these methods for testing cement-based composites has been recently presented by Shah and Ribakov (2011). In this section, a brief review of acoustic emission, ultrasonic pulse velocity and microscale X-ray computed tomography techniques is presented.
2.7.1 Acoustic emission and ultrasonic pulse velocity
The acoustic emission (AE) technique allows the characterisation of damage evolution in concrete materials at the structural scale. According to this technique, transient waves generated by crack propagation are recorded by sensors placed at the surface of the specimen; then an appropriate AE descriptors are used to characterise and quantify the level of the damage inside the specimen, and the location of the cracks. The shape of the AE waveforms is closely connected to the fracture mode. Shear events are recognised by longer rise time and high amplitude than tensile events (Ohtsu et al., 2007). AE has been used to characterise the damage process of FRC beams during four-point bending tests (Aggelis et al., 2011) and to investigate the effect of chemically treated steel fibres on the fracture behaviour of the FRC beams (Aggelis et al., 2012). It was found that chemically treated fibres induce further matrix cracking, due to stronger bonding to the matrix, than untreated fibres. AE was also used to study the effect of fibre content on the fracture mode of FRC beams (Soulioti et al., 2009), and to study early-age cracking (Kim & Weiss, 2003). Rouchier et al. (2013) used both digital image correlation and AE to monitor damage in FRC during tensile loading tests. However, there are difficulties in interpreting the results obtained from AE, as it is unable to differentiate between acoustic emissions caused by different mechanisms taking place during crack propagation in FRC such as: matrix cracking patterns, fibre debonding and fibre pull-out (Mobasher et al., 1990).

Ultrasonic Pulse Velocity (UPV) is another non-destructive method, that can be used to determine the elastic properties of FRC (Benaicha et al., 2015; Hassan & Jones, 2012; Washer et al., 2005). The velocity of waves in a material depends mainly on the material's elastic properties and its density. It can be also used to assess damage and quantify its extent in different concrete structures (Mirmiran & Wei, 2001; Shah & Hirose, 2009). This tool is useful to quantify the extent of damage after a mild earthquake (Shah & Ribakov, 2011).

2.7.2 Microscale X-ray computed tomography
The microscale X-ray computed tomography (µXCT) is a non-destructive 3D imaging technique that allows accurate characterisation of the 3D nano-/micro-/meso-structure of
different types of materials including pores and cracks. Computed tomography has been used in medicine since 1970s, however, its application in material science is relatively new. It is being increasingly used to evaluate damage propagation, identify damage mechanisms and extract key parameters of different types of materials (Maire and Withers, 2014). This can be achieved through recording several scans at different time intervals under changing conditions, and then comparing the successive 3D images to quantify structural evolution in the material. This approach, sometimes described as 4D imaging (Maire & Withers, 2014), allows the investigation of several phenomena at small scales. A comprehensive review of the application of µXCT in material science was presented by Stock, (1999, 2008) and Maire and Withers (2014). A few studies have applied µXCT on FRC, focusing mainly on characterising the fibre orientations within the concrete/mortar matrix (Barnett et al., 2010; Suuronen et al., 2012); determining fibre spacing and 3D porosity (Ponikiewski et al., 2015a, 2015b) and measuring fracture energy released by various failure mechanisms (Trainor et al., 2013). Qsymah et al. (2015) has recently used µXCT to characterise the internal structure of a single UHPFRC specimen (specifically, fibres and pores) and used the obtained data to develop an image-based finite element models to predict the effective elastic properties of UHPFRC. To date, the evolution of the toughening mechanisms of a cementitious composite, reinforced with short random fibres, has not been studied non-destructively using µXCT to the best knowledge of the author. A brief review on the procedures of the µXCT tests is presented below.

2.7.2.1 µXCT principles

Figure 2.7 illustrates the procedures of the µXCT (Kruth et al., 2011; Landis et al., 2003). A sample is placed between the X-ray source and a detector. As the X-rays propagate through the sample, which is rotated axially through 360°, they are attenuated or scattered depending on the density of the sample along the beam path. The remaining X-rays transmitted through the sample are captured by the detector, and then used to build a series of 2D digital radiographs (projections). Using a suitable reconstruction algorithm, a 3D volumetric image of the sample with variable greyscale is then reconstructed from the radiographs. The grey values of each voxel (3D pixels) are a measure of the absorptivity of the material.
The X-ray radiation is characterised by its energy distribution (measured in kV) and intensity, which determine the penetrating power of the X-ray beam into a material. Higher energy X-rays can penetrate a greater thickness of the material, or a similar thickness of denser material before being absorbed. However, high energy X-rays are less sensitive to the differences in the densities of the material constituents. Therefore, the energy of the X-ray beam should be calibrated carefully according to the sample size and the density of the material, to ensure the quality of the scanned images. It is essential to have small electron beam or X-ray spot to obtain sharp images. Spots of around 1µm diameter can be achieved with an applied voltage up to 250kV. The material composition and its attenuation coefficient have also a great effect on the quality of the µXCT images (Kruth et al., 2011).

At the beginning of the scan, the size of the image voxels should be calibrated in order to perform accurate and traceable dimensional measurements. This calibration allows identification a global scale factor that will be used to link voxel size to unit of length. The calibration process is usually done by measuring a simple calibrated reference object.

In addition, a large number of parameters, which have great influence on the scanning
process, need to be determined at the beginning of the scan such as: source current, source voltage, the size and shape of the object, magnification, number of angular poses, exposure time, number of projections, number of positions and combining measurements with different current/voltage/target. Proper selection of these parameters may need iterative procedures and test measurements (Ketcham & Carlson, 2001; Kruth et al., 2011).

2.7.2.2 Data reconstruction and segmentation

Image reconstruction is a mathematical process that aims to convert projection images collected by the detector into greyscale images. The grey values have a range determined by the computer system (e.g., 8-bit). The most commonly used reconstruction technique is called filtered back projection, in which each view is successively superimposed over a square grid in the direction it is originally acquired. The resolution of the reconstruction are affected by many parameters such as: voxel size, number of detector pixels in x and y directions, number of angular positions at which images are taken and number of projection images taken in one angular pose (Ketcham & Carlson, 2001).

The 3D reconstruction is followed by edge detection and segmentation, to determine the interfaces between the object and the surrounding air or between different material components. The object sample or material edges can be identified based on greyscale value thresholding. The edge grey value depends on the material quality as well as the radiation intensity. Proper edge detection is complicated by the presence of multiple materials. The threshold values can be calculated and applied on local transition area that includes only the two materials considered for the transition threshold, rather than applying the same threshold value over the entire sample (i.e., global thresholding). However, this requires long procedures to identify accurate threshold values (Kruth et al., 2011).

2.8 Summary

The superior properties of UHPFRC make this material suitable for many structural applications. The application of UHPFRC is usually combined with extensive experimental tests to ensure that its properties are optimised and achieved. Modelling UHPFRC at the mesoscale allows investigation of the effect of meso-structure on
UHPFRC behaviour at the macroscale, and thus can be used to optimise the material properties without costly experimental work. A few studies have proposed mesoscale models of the FRC, in which the material's internal structure is generated using statistical algorithms with inclusions of simplified shapes and assumed distributions. The review of the existing models reveals that there is a lack of robust and accurate models for UHPFRC that can link the realistic material micro-/meso-structures and its mechanical properties at macroscale.

The application of non-destructive testing techniques on FRC allows for better understanding of the material behaviour and properties. One of the most powerful non-destructive tools that can be applied on FRC is μXCT, which provides accurate 3D images of the internal micro-structure of the material. These images can be used to characterise the material's behaviour under variable conditions, and to develop numerical models with faithful representation of the material internal structure. Such models may offer a practical tool for designers to optimise the material internal structures. However, in-situ μXCT tests of UHPFRC specimens under progressive loadings have not been reported.
Chapter 3: 2D Mesoscale FE Model of UHPFRC Using Cohesive Interface Elements

In this chapter, 2D mesoscale finite element models were developed to simulate the complicated fracture behaviour of UHPFRC by considering it as a three-phase material: the mortar matrix, the steel fibres and the fibre-mortar interfaces. Discrete cracks in the mortar were modelled by pre-inserted zero-thickness cohesive interface elements inside the solid elements. The fibres were generated in an in-house Matlab code with random distribution. Each fibre was split into several segments at the intersections with the cohesive elements in mortar, and each segment was modelled as a two-noded 1D element. The fibre-mortar interfaces were modelled using nonlinear spring-like connector elements, that connect the fibre segments and bridge the crack surfaces. The constitutive behaviours of these connector elements were determined by a micro-mechanical model. The mesoscale models were validated against direct tensile tests and parametric studies were conducted for the effects of the content, length and orientation of fibres on the tensile fracture behaviour.

3.1 Modelling the mortar matrix using cohesive elements

3.1.1 Generating the mesh with cohesive elements

The mortar matrix was first meshed in ABAQUS/CAE using 2D plane stress elements. The mesh data was then input into a Matlab code developed by Yang, Su, et al. (2009) for inserting of four-noded cohesive interface elements (CIEs) into the initial mesh. Figure 3.1 illustrates the method of inserting CIEs. In the case of four-noded plane stress elements, each node was replaced by four separated nodes at the same position. Four CIEs of element type COH2D4 in ABAQUS were generated along the common element edges. After inserting CIEs, the input file with both solid elements and cohesive elements was re-written.
3.1.2 Cohesive elements in ABAQUS
The constitutive behaviour of CIEs was modelled by linear traction-displacement softening laws. Figures 3.2a and b illustrate these laws for both normal and tangential tractions versus relative displacements of the crack surfaces. The initial response in these curves is linear, representing the initially un-cracked material. In 2D problems, the interfacial separation represents the crack opening displacement $\delta_n$ and the crack sliding displacement $\delta_s$, corresponding to normal $t_n$ and shear tractions $t_s$, respectively. The unloading curves are also shown in Figures 3.2. The initial tensile stiffness $k_{n0}$ and the initial shear stiffness $k_{s0}$ should be high enough to represent the un-cracked material, but not too high to cause numerical ill-conditioning. Proper values for $k_{n0}$ and $k_{s0}$ can be determined by trial and error (Chandra et al., 2002; Yang, Su, et al., 2009).
Figure 3.2 Typical linear tension softening curves for the cohesive element (Yang, Su, et al., 2009).

The cohesive element COH2D4 in ABAQUS is based on the above cohesive crack model (ABAQUS, 2012). In this element the stiffness $k_n$ and $k_s$, upon unloading and reloading, are degraded with the increase of the interfacial separation $\delta_n$ and $\delta_s$ due to irreversibly progressive damage. The overall damage of the crack is represented by a scalar index $d$ (defined in equation 3.3 below) which is function of the effective relative displacement $\delta_m$:

$$\delta_m = \sqrt{(\delta_n)^2 + \delta_s^2}$$  \hspace{1cm} (3.1)

where $\langle \Delta \rangle$, the Macaulay brackets, is defined as:

$$\langle \delta_n \rangle = \begin{cases} \delta_n, & \delta_n \geq 0 \text{ (tension)} \\ 0, & \delta_n < 0 \text{ (compression)} \end{cases}$$  \hspace{1cm} (3.2)

In the case of linear softening law, the damage $d$ evolves according to:

$$d = \frac{\delta_m(f(\delta_{m,max} - \delta_{m0}))}{\delta_{m,max}(\delta_{mf} - \delta_{m0})}$$  \hspace{1cm} (3.3)

where $\delta_{m,max}$ is the maximum effective relative displacement attained during the loading history, $\delta_{m0}$ and $\delta_{mf}$ are effective relative displacements at damage initiation and complete failure respectively.

The stiffness $k_n$ and $k_s$ are computed as:

$$k_n = (1 - d)k_{n0}$$  \hspace{1cm} (3.4)

$$k_s = (1 - d)k_{s0}$$

and the tractions as:

$$t_n = \begin{cases} (1 - d)t_n', & t_n' \geq 0 \\ t_n', & t_n' < 0 \text{ (No damage to compressive stiffness)} \end{cases}$$  \hspace{1cm} (3.5)
where \( t'_{n} \) and \( t'_{s} \) are the traction components predicted by the elastic traction-separation behaviour for the current separation without damage.

Several damage initiation criteria, which refer to the beginning of the stiffness degradation at a material point, are available in ABAQUS. Herein, the damage was assumed to initiate when a quadratic interaction function involving the nominal stress ratios reaches the unit value (ABAQUS, 2012):

\[
\left( \frac{t_n}{t_{n0}} \right)^2 + \left( \frac{t_s}{t_{s0}} \right)^2 = 1
\]  
(3.6)

Once the damage initiation criterion is met, damage propagates according to the damage evolution law described in equation (3.3).

### 3.2 Modelling the fibre phase

#### 3.2.1 Generating the random fibre distribution

The UHPFRC is usually reinforced with a large number of short steel fibres distributed randomly in the mortar matrix. The orientation of the random fibres is commonly quantified through “orientation factor \( \eta_i \)” defined as (Abrishambaf et al., 2013; Soroushian & Lee, 1990):

\[
\eta_i = \frac{1}{N_f} \sum_{f=1}^{N_f} |\cos \phi_{if} | 
\]  
(3.7)

where \( i = 1, 2, \) and 3 corresponding to \( x-, y- \) and \( z- \)axes, \( \phi_{if} \) is the orientation angle of the \( f^{th} \) fibre with respect to the axis \( i \) and \( N_f \) is the total number of fibres. \( \eta_i \) varies from 0 to 1. The value 1 represents totally aligned fibres, while the value 0 indicates that all the fibres are oriented perpendicular to the direction considered. It is 0.5 when the distribution is isotropic.

The randomly distributed 1D fibre elements were generated statistically using a Matlab code developed by Su et al. (2011) based on a random sequential addition algorithm. In
this algorithm fibres with a prescribed length are added to a region by randomly defining the two-end nodes in the global coordinate system, until a target volume fraction is achieved. To keep both ends of the fibres within the specimen, fibres crossing the boundaries are discarded from the model. As a result, the fibre density near the boundaries is slightly lower than that in the middle region, and the majority of fibres near boundaries tend to align parallel to the boundaries. This tendency increases when long fibres are modelled, as shown later in section 3.4.2.

3.2.2 Modelling the fibre-matrix interface

The Matlab code for generating fibre elements was combined with that for inserting CIEs, and then further developed in this study to consider the fibre-mortar interfaces. This was done using nonlinear spring-like connector elements as illustrated in Figure 3.3. The resulting Matlab code involves the following procedure:

1. generate the mesh for the mortar in ABAQUS/CAE and then import the input file of this mesh into Matlab to insert CIEs as described in section 3.1.1;

2. generate random 1D fibre elements until a target volume fraction is achieved as described in section 3.2.1;

3. determine the intersection points between the fibres and the cohesive elements, and split the fibres at these points. Figure 3.3a shows a fibre crosses two CIEs was split into three segments. A single fibre may cross many cohesive elements, depending on the size of the mortar mesh. Each fibre segment was modelled as a truss element T2D2 (ABAQUS, 2012), and perfectly bonded with the mortar mesh;

4. determine the orientation angles ($\phi$) and the embedment length ($l_e$) of each fibre. $\phi$ is defined here as the angle between a fibre and the normal to the crack surface as seen in Figure 3.3b. $l_e$ is the shorter distance between the intersection with the crack surfaces and the fibre ends;

5. insert connector elements between the segments of each fibre at each intersection as shown in Figure 3.3c (connector elements are in red);
(6) find the unique pull-out curve of each fibre as function of its orientation angle ($\phi$) and its embedded length ($l_e$), and assign these curves to the corresponding connector elements. The pull-out behaviours were defined using the analytical pull-out model presented in the next section;

(7) complete the finite element model by defining the analysis step, embedded regions, applied load, boundary conditions, etc, and import it back into ABAQUS for analysis.

The connector element CONN2D2 with the connection type AXIAL in ABAQUS was used in this model. The AXIAL connector provides a connection between two nodes and transfer forces along the line connecting the nodes. It has an advantage over the conventional spring element in that it can be used to define several material-like behaviours like elasticity, plasticity, damage and failure by describing its constitutive law in series. Moreover, connector elements can be used in both implicit and explicit solvers in ABAQUS, whilst spring elements can be used in the implicit solver only. Their constitutive responses are described in terms of force (corresponding here to the pull-out force) versus displacement (corresponding to the fibre slip). In the next section, the analytical pull-out model used to calculate the pull-out curves of fibres is presented.

### 3.2.3 Pull-out behaviour of fibres

Generally, the pull-out curves used in mesoscale models to simulate fibre-mortar interface are either calculated using analytical pull-out models (Bolander & Saito, 1997;
Kabele, 2007; Radtke et al., 2010; Schaufler & Cusatis, 2011), or determined experimentally by pull-out tests (Cunha et al., 2012; Kunieda et al., 2011). The stress-based analytical pull-out model proposed by Naaman et al. (1991a, 1991b) was used here to determine the pull-out curves of each fibre. Figure 3.4 shows the bond stress-slip relation for straight smooth fibres used by Naaman et al. (1991a) to find the analytical pull-out force-displacement curve of short steel fibres. Basically, this relation is the constitutive behaviour of the interface and thus preferable as an input in the FE models for UHPFRC. However, the pull-out curve can be also used to perform the analysis (Bolander & Saito, 1997). The Naaman's model was extended by Lee et al. (2010) to consider the effect of fibre orientation angle of inclined steel fibres in UHPFRC specimens. In this section, the basic equations of this model are presented. For the complete mathematical derivation one can refer to Naaman et al. (1991a, 1991b) and Lee et al. (2010).

![Figure 3.4](image)

Figure 3.4 Typical interfacial bond shear stress versus slip (Naaman et al., 1991a).

Figure 3.5 shows a typical pull-out load versus end slip curve for a fibre. The initial part of this curve describes the linear elastic behaviour of the fibre-matrix interface when the fibre is completely bonded along its length with the surrounding matrix. The displacements of the fibre and the matrix at the interface remain compatible, and the pull-
out curve is linear elastic up to the critical load $P_{\text{crit}}$, which can be defined as function of the fibre orientation angle $\phi$ using:

$$P_{\text{crit}}(\phi) = \frac{\pi d_f \tau_{\text{max}}(\phi)}{\lambda} \left[ \frac{1 - e^{-2\lambda \Delta_e}}{(1 - \frac{1}{Q})(1 + e^{-2\lambda \Delta_e}) + \left(\frac{1}{Q}\right)2e^{-\lambda \Delta_e}} \right]$$  \hspace{1cm} (3.8)

where $\lambda = \sqrt{KQ}$, $K = \frac{\pi d_f \kappa}{A_m E_m}$, and $Q = 1 + \frac{A_m E_m}{A_f E_f}$.

$\tau_{\text{max}}$ is the average bond shear stress, $\kappa$ is the initial slope of the bond-slip curve shown in Figure 3.4 and called bond modulus, and $A$ and $E$ are the cross sectional area and modulus of elasticity respectively, where the subscript $f$ and $m$ stands for fibre and matrix respectively.

![Figure 3.5 Typical pull-out curve of a smooth fibre (Naaman et al., 1991a).](image)

In the case of inclined fibres, the snubbing effect and matrix spalling are introduced to the bond stress ($\tau$) by (Lee et al., 2010; Li et al., 1991):

$$\tau(\phi) = e^{f \phi}(\cos \phi)^{\omega \tau(\phi = 0)}$$  \hspace{1cm} (3.9)
For UHPFRC with short steel fibres, the snubbing coefficient $\hat{f}$ and the spalling coefficient $\omega$ are assumed as 1.6 and 1.8 respectively, following Lee et al. (2010). The effects of snubbing and matrix spalling on the slip value ($\Delta$) are considered by introducing the coefficient $\beta$ as follows (Lee et al., 2010):

$$\Delta(\phi) = \beta \Delta(\phi = 0)$$ \hspace{1cm} (3.10)

where

$$\beta = 1 + \gamma \left( \frac{2\phi}{\pi} \right)^{\xi}$$ \hspace{1cm} (3.11)

The values of $\xi$ and $\gamma$ can be determined by comparing the results of these equations with experimental curves. For UHPFRC, Lee et al. (2010) found that $\xi = 2$ and $\gamma = 100$.

The pull-out curve is calculated in three different stages as follows:

**Perfectly bonded region:** when $P \leq P_{crit}$, the fibre is perfectly bonded to the surrounding matrix. The pull-out curve is linear and its slope is defined by:

$$\frac{P}{\Delta(\phi)} = \frac{1}{\beta} \frac{\lambda A_m E_m}{Q - 1} \frac{1 + e^{-\lambda l_e}}{1 - e^{-\lambda l_e}}$$ \hspace{1cm} (3.12)

**Partially debonded region:** when the applied load exceeds the critical load ($P_{crit}$), the debonded zone develops and grows as the applied force increases. Thus, part of the fibre is debonded from the matrix, while the other part is still fully bonded. Here, the pull-out load $P$ is balanced by the resistance of the fibre in the debonded zone $P_d$ and that in the bonded zone $P_b$ as:

$$P = P_b + P_d$$ \hspace{1cm} (3.13)

The length of the debonded zone is denoted by $z$, thus the length of the bonded zone is $(l_e - z)$. The debonded length $z$ increases from zero at the onset of debonding to the initial embedded fibre length $l_e$ at full debonding. The pull-out load and the corresponding slip displacement in this stage can be calculated by:
where $\tau_f$, the frictional bond stress, is equal to $\tau_{\text{max}}$ for UHPFRC (Lee et al., 2010).

**Fully debonded region:** in this stage the fibre starts to pull-out, and the following equations hold:

\[
P(\phi) = \pi d_f \tau_f(\phi)z + \frac{\pi d_f \tau_{\text{max}}(\phi)}{\lambda} \times \frac{1 - e^{-2\lambda(l_e - z)}}{\left(\frac{2}{Q}\right)e^{-\lambda(l_e - z)} + \left(1 - \frac{1}{Q}\right)(1 + e^{-2\lambda(l_e - z)})}
\]

\[
\Delta(\phi) = \frac{\beta}{A_m E_m} \left\{ P(\phi)(Q - 1)z - \frac{\pi d_f \tau_f(\phi)z^2}{2}(Q - 2) + (P(\phi) - \pi d_f \tau_f(\phi)z) \frac{1 - e^{-\lambda(l_e - z)}}{1 + e^{-\lambda(l_e - z)}} \frac{Q - 2}{\lambda} \right\}
\]

where $\Delta$ is a constant determining the initial slope of the frictional slip behaviour, $\rho$ is a constant related to the shape of the exponentially descending branch of the bond slip curve, $\Delta_0$ is the end slip of the fibre at full debonding, $\mu$ is the friction coefficient on the fibre-matrix interface, $\nu$ is the Poisson's ratio and $\dot{x}$ is the embedded length that varies from $l_e$ to zero.

It has been found that the pull-out behaviour of a fibre embedded in a plain matrix is different from a fibre embedded in a fibre reinforced matrix. Several researchers have
investigated the influence of fibre volume fraction in the matrix on the pull-out behaviour of steel fibres (Markovic, 2006; Shannag et al., 1997; Yoo et al., 2013). They found that the average bond strength of fibre embedded in a plain concrete matrix is about 13-33% lower than that of fibre embedded in a composite matrix with fibre volume fractions of 1-4%. Based on these findings, Kang and Kim, (2011) proposed a magnifying parameter $\alpha_f$ to take account of this effect as:

$$P_c(\phi, l_e, \Delta) = \alpha_f P(\phi, l_e, \Delta)$$

(3.18)

where $\alpha_f = 1.25$ is adopted here as in (Kang & Kim, 2011).

3.3 Modelling of a direct tension test and validation

The proposed model was validated against the direct tensile test conducted by Hassan et al. (2012) for the dog-bone UHPFRC specimen shown in Figure 3.6a. The middle prism of the specimen (100×26×50mm) was modelled (Figure 3.6b). The left edge was fixed in horizontal and vertical displacements (Figure 3.6b). The tension was applied by displacement-control with a uniformly distributed displacement (max 6mm) applied to the nodes on the right edge.

Straight steel fibres are of 2% in volume fraction, 2000MPa in strength, 0.2mm in diameter and 13 mm in length. The number of fibres $N_f$ was calculated by:

$$N_f = \text{int} \left[ \frac{4f_f V}{\pi d_f^2 l_f} \right]$$

(3.19)

where $f_f$ is the volume fraction of fibres and $V$ is the volume of the specimen. There are $N_f=6370$ fibres in the middle prism shown in Figure 3.6b.
a) The dog-bone specimen tested by Hassan et al. (2012).

b) The middle prism used in the model, the boundary conditions and load.

Figure 3.6 Modelling direct tensile test of UHPFRC specimen tested by Hassan et al. (2012), dimensions in mm.

The specimen was modelled first with a single pre-defined crack at the middle of the dog-bone specimen by inserting CIEs in one vertical line crossing the whole specimen as shown in Figure 3.7. Fibres crossing the CIEs were split at the intersection with the crack, and connector elements were inserted between the fibre elements to connect the inner nodes of the split fibres and bridge the cohesive elements as shown in Figure 3.7. The 6730 fibres were modelled using 7383 truss elements, with 653 fibres split into two elements and 653 connector elements inserted. The mortar matrix was modelled by 165 reduced-integration plane stress elements (CPS4R) and seven CIEs (COH2D4). The total number of nodes in the model was 13974. The fibre elements were perfectly bonded with the mortar mesh using the command "*EMBEDDED ELEMENT" in ABAQUS.
The fibres and mortar were modelled as a linear elastic material. The elastic moduli were 200GPa and 42.08GPa and the Poisson's ratio were 0.3 and 0.18, respectively. The tensile strength of the mortar was 5.36MPa (Hassan et al., 2012). The elastic stiffness of the cohesive elements $k_{n0}$ and $k_{s0}$ (see Figure 3.2) in this model was determined by examining several values starting from the elastic modulus of the mortar matrix as follows: 4.0E+1; 4.0E+2; 4.0E+3; and 4.0E+4 GPa/mm. It was observed that as the value of the elastic stiffness decreases, the pre-peak slope of the predicted tensile stress versus displacement curve were decreased. Using higher values is not acceptable for a complete FE simulation. Thus, the value of 4.0E+4 GPa/mm was found reasonable and used in all the models developed in this chapter.
The mix design used by Hassan et al. (2012) is similar to that used by Lee et al. (2010) in pull-out tests with same properties for the steel fibres. Therefore, the bonding properties in this FE model were extracted from the experimental data in Lee et al. (2010), and used to calculate the 3-stage pull-out curves in the Naaman's model (equations 3.12-3.17) which were then assigned to the connector elements as elastic-plastic constitutive behaviour. The mortar fracture energy was assumed equal to 30J/m² (Richard & Cheyrezy, 2011). Table 3.1 shows all the model parameters. The simulation was carried out using ABAQUS/standard version 6.12 as a static stress analysis.

Table 3.1 The parameters used in the direct test model for UHPFRC.

<table>
<thead>
<tr>
<th>Parameters used in modelling</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus of the fibres, GPa</td>
<td>200</td>
</tr>
<tr>
<td>Poisson's ratio of fibres</td>
<td>0.3</td>
</tr>
<tr>
<td>Tensile strength of the steel fibres, MPa</td>
<td>2000</td>
</tr>
<tr>
<td>Young's modulus of mortar matrix, MPa</td>
<td>42.08</td>
</tr>
<tr>
<td>Poisson's ratio of mortar matrix</td>
<td>0.18</td>
</tr>
<tr>
<td>Fracture energy of mortar matrix, J/m²</td>
<td>30</td>
</tr>
<tr>
<td>Tensile strength of mortar matrix, MPa</td>
<td>5.36</td>
</tr>
<tr>
<td>Bond strength ($\tau_{\text{max}}$), MPa</td>
<td>6.80</td>
</tr>
<tr>
<td>Bond modulus ($\kappa$), MPa/mm</td>
<td>4000</td>
</tr>
<tr>
<td>Coefficient of friction, $\mu$</td>
<td>0.3</td>
</tr>
<tr>
<td>Coefficient of exponential shape of the descending branch ($\rho$)</td>
<td>0.05</td>
</tr>
<tr>
<td>Snubbing friction coefficient, $\hat{f}$</td>
<td>1.6</td>
</tr>
<tr>
<td>Spalling coefficient, $\omega$</td>
<td>1.8</td>
</tr>
<tr>
<td>Parameters used to calculate $\beta$ in equation (3.11), $\xi$ and $\gamma$</td>
<td>2, 100</td>
</tr>
</tbody>
</table>

Figure 3.8 compares the numerical tensile stress-displacement curve with the experimental data in (Hassan et al., 2012). It can be seen that the agreement between the
two curves is good. Nevertheless, the numerical response exhibits a sudden drop and recovery after the ultimate tensile stress due to the failure of the CIEs, leaving fibres to resist the applied load alone at the post peak stage. However, the tension softening behaviour of mortar matrix in a real UHPFRC specimen occurs very slowly due to the presence of fibres, which arrest cracks in the matrix leading to multiple cracking behaviour (Qsymah et al., 2016). The mechanism of arresting cracks in the matrix cannot be modelled in this single crack model.

Figure 3.8 Comparison between the numerical and experimental tensile response.

**3.4 Parametric study**

The same FE model in Figure 3.7 was then used to perform parametric studies on the effects of content, length and orientation of fibres on the tensile behaviour of UHPFRC. While a parameter is studied, all other parameters remain the same as in Table 3.1.

**3.4.1 Effect of fibre content**

The influence of fibre volume fraction is shown in Figure 3.9. The volume fractions used were: 0.5%, 1%, 1.5%, 2% and 3%. It can be seen that, as the fibre content increases, the peak stress and the dissipated fracture energy (described by the area under the curve) increase significantly. The predicted tensile strengths were 6.15, 7.43, 8.21, 9.05 and 13.33MPa for fibre volume fractions 0.5%, 1%, 1.5%, 2% and 3% respectively. The
increase in the tensile strength due to higher fibre content has been shown experimentally (Markovic, 2006; Yoo et al., 2013). However, using too high fibre content may reduce the tensile strength of the UHPFRC due to fibre interaction with each other (Le, 2008). The fibre interaction was not considered in these models.

3.4.2 Effect of fibre length

Figure 3.10 plots the numerical tensile responses for the UHPFRC specimen with 2% fibres having lengths of: 10, 13, 15, 18 and 20mm. The results show that longer fibres leads to higher peak tensile stress and fracture energy. This can be due to two reasons: The first is that longer fibres have higher bridging forces (Li et al., 1991). The second is that longer fibres tend to orient along the specimen length (parallel to the direction of applied load in this case) due to boundary effect in random generation (Soroushian & Lee, 1990). Therefore, the number of fibres crossing the crack plane (fibre density) and the orientation factor of longer fibres relative to the direction of applied load increase for longer fibres. Table 3.2 shows the orientation factors and the fibre densities at the crack plane for different fibre lengths. The orientation factor increases to 0.74 for 20mm fibre length from 0.63 for 10mm fibre length, while the fibre density at the crack plane rises from 0.35 to 0.85 fibre/mm².
The critical fibre length calculated for the modelled fibres using equation 2.4 (section 2.2.2) is equal to 14.7mm (with 0.2mm diameter and 2000MPa tensile strength). According to this equation, fibres longer than the twice of the critical length are more likely to rupture rather than to pull-out (Li et al., 1990). However, the possibility of fibre rupture was not considered in this model.

![Graph showing the effect of fibre length on the tensile behaviour of the UHPFRC with constant fibre volume fraction (2%).](image)

**Figure 3.10** The effect of fibre length on the tensile behaviour of the UHPFRC with constant fibre volume fraction (2%).

Table 3.2 The orientation factors and fibre densities at the crack plane for the UHPFRC specimens with different fibre lengths.

<table>
<thead>
<tr>
<th>Fibre length (mm)</th>
<th>Orientation factor</th>
<th>Fibre areal density (fibre/mm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.74</td>
<td>0.85</td>
</tr>
<tr>
<td>18</td>
<td>0.72</td>
<td>0.72</td>
</tr>
<tr>
<td>15</td>
<td>0.70</td>
<td>0.58</td>
</tr>
<tr>
<td>13</td>
<td>0.67</td>
<td>0.45</td>
</tr>
<tr>
<td>10</td>
<td>0.63</td>
<td>0.35</td>
</tr>
</tbody>
</table>
3.4.3 Effect of fibre orientation

A specimen with randomly distributed fibres (orientation factor relative to the loading direction $\eta_1=0.67$), and another with all fibres aligned with the loading direction ($\eta_1=1$), shown in Figure 3.11a and b were modelled. As shown in Figure 3.12, the specimen with aligned fibres is much stronger than that with randomly distributed fibres (ultimate tensile strength are 9.01MPa and 15.53MPa, respectively). These results are in good agreement with experimental results in (Barentt et al., 2010; Kang & Kim, 2011). This indicates the importance of considering realistic fibre orientations in numerical modelling.

Figure 3.11 The UHPFRC specimen with randomly distributed and aligned fibres (in red).
3.5 Modelling multiple cracking behaviour of UHPFRC

The specimen (shown in Figure 3.7) was re-simulated by inserting CIEs between all edges of the mortar elements to model the multiple cracking behaviour of UHPFRC. Connector elements were also inserted between fibre elements at all intersections with the CIEs. To reduce the computational time, the model has 1000 fibres (with $f_i=0.33\%$). All model parameters were kept the same as in Table 3.1.

From Figure 3.13 it can be seen that there is a slight increase in the tensile strength (5.54 MPa) over that of the unreinforced mortar (5.36 MPa) due to the low fibre content. Figure 3.14 shows the cracking process at different loading stages in terms of stiffness degradation variable (SDEG). The red elements represent the elements that are completely failed with SDEG close to 1. The specimen experienced multiple cracking behaviour as seen in Figures 3.14 a, b and c, followed by the a macro-crack (Figure 3.14d) while other cracks closed.

This model suffers from the possibility of forming several localised macro-cracks at different locations at the same time. This problem can be tackled by developing subroutines in ABAQUS that can extract the crack width at different locations and update
the constitutive laws of the connector elements according to the crack widths. Also, to model the arresting of cracks in the matrix a very fine mesh is required, resulting in unpractical model in which fibres could be split into a large number of quite small 1D elements and a large number of connector elements.

Figure 3.13 The predicted tensile behaviour from a multiple cracking model for a UHPFRC specimen reinforced with 1000 fibres.
a) Displacement = 0.04mm, deformation scale factor = 150.

b) Displacement = 0.05mm, deformation scale factor = 150.

c) Displacement = 0.08mm, deformation scale factor = 150.

d) Displacement = 6mm, deformation scale factor = 1.

Figure 3.14 Multiple cracking behaviour of UHPFRC reinforced by 1000 fibres at different loading stages.
3.6 Summary

This chapter has presented 2D mesoscale FE models to simulate the tensile fracture behaviour of UHPFRC. Discrete cracks in the mortar were modelled using CIEs that were inserted inside the mortar solid elements. Fibres were modelled as two-noded 1D random elements that are not related to the mortar mesh, and each fibre was split into segments at the intersections with the CIEs. The pull-out behaviour of fibres was modelled using connector elements that connect the fibre segments and bridge the CIEs.

The numerical results are in reasonable agreement with the experimental data. Parametric studies show that increasing the fibre contents and lengths leads to higher tensile strength and fracture energy. It is also shown that the fibre orientation greatly affects the tensile behaviour of the UHPFRC and should be considered in mesoscale modelling.
Chapter 4: In-Situ Micro X-Ray Computed Tomography Tests of UHPFRC

This chapter presents in-situ micro X-ray computed tomography (µXCT) tests of notched UHPFRC specimens under wedge split loading. A sequence of tomography absorption contrast images were first acquired at different loading stages, which were then processed to characterise the material's internal structure and to study the evolution of matrix cracking and toughening mechanisms in UHPFRC during loading. Mechanisms like crack arresting, fibre pulling out, fibre bending and mortar spalling at fibre exit points were visualised and discussed by 2D images and 3D volume rendering. The number of the effective fibres in at the cracking plane was determined and the load vs. crack width at the notch tip relationship was extracted using the µXCT images. The porosity and the fibre orientation of the UHPFRC specimen used in the first in-situ test were also analysed.

4.1 Experiments

µXCT has been used to visualise and analyse the internal micro-structures of many composites. However, very limited studies have combined this imaging technique with in-situ loading tests. In this study, in-situ wedge splitting tests with µXCT were conducted on two 20x25x40mm UHPFRC specimens. The wedge splitting test was selected because it is simple and stable fracture test (Karihaloo et al., 2003; Rossi et al., 1991; Walter et al., 2005).

4.1.1 Material and specimens

The mix design of UHPFRC investigated in this study, summarised in Table 4.1, was developed at the University of Liverpool (Hassan et al., 2012; Le, 2008; Yang, Millard, et al., 2009), where the detailed fabrication process could be found. The mortar has a high content of Portland cement (CEM 1) superfine silica fume, ground granulated blast-furnace slag (GGBS) and silica sand with 0.27mm average diameter. No coarse aggregate were used. The water to binder ratio was 0.15. A high dosage of water reducing admixture was added to the mix to get proper workability. The mortar was reinforced with 2% straight steel fibres of 13mm in length, 0.2mm in diameter, 2000MPa in strength and 200GPa in elastic modulus. The basic properties of the material at 28 days from
standard tests are (Hassan et al., 2012): compression strength 150.56MPa, tensile strength 9.07MPa, and Young's modulus 45.55 GPa. They are 121.32 MPa, 5.36 MPa and 42.08GPa, respectively for the ultra high performance concrete without steel fibres.

Table 4.1 Details of the UHPFRC mix (Hassan et al., 2012).

<table>
<thead>
<tr>
<th>Mix content</th>
<th>Kg/m³</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cement</td>
<td>657</td>
</tr>
<tr>
<td>Ground Granulated Blast Furnace Slag</td>
<td>418</td>
</tr>
<tr>
<td>Microsilica (Silica Fume)</td>
<td>119</td>
</tr>
<tr>
<td>Silica Sand (average diameter 0.27mm)</td>
<td>1051</td>
</tr>
<tr>
<td>Superplasticizer</td>
<td>40</td>
</tr>
<tr>
<td>Water</td>
<td>185</td>
</tr>
<tr>
<td>Steel fibre, $f_f=2%$</td>
<td>157</td>
</tr>
</tbody>
</table>

The specimens used in this test were cut from one of the UHPFRC beams cast for a size-effect investigation (Mahmud et al., 2013). Several specimens were tested first mechanically (without $\mu$XCT scanning) to determine the proper dimensions for the in-situ tests based on two considerations. On the one hand, the specimen should be large enough to permit a representative crack development. On the other, it should be small enough to achieve sufficient image resolution for crack detection. The determined dimensions of the specimens were 40x25x20mm, with a groove and a 8mm deep notch (Figure 4.1a).

4.1.2 Loading system

A special loading wedge system, shown in Figure 4.1, was designed and made at the structural laboratory in University of Manchester. The wedge angle is 17° (Figure 4.1b). Two steel loading rollers (rods) are placed inside the groove and welded with steel angles that are mounted on the top of the specimen to keep them fixed during the test (Figure 4.1c). Moving the wedge vertically downwards creates a force ($F$) which applies two horizontal splitting components ($F_1$) at the loading rollers (Figure 4.1d). The specimen was mounted on two parallel supports.
a) UHPFRC specimen used in the in-situ test (dimensions in mm).

b) Wedge with angle $17^\circ$.

c) Loading rollers and two line supports.

d) Load transfer.

Figure 4.1 Setup of the wedge splitting tests and specimen's dimension.

4.1.3 In-situ $\mu$XCT tests and image acquisition

These in-situ tests were carried out at Henry Mosley X-ray Imaging Facility (University of Manchester, UK), using the 225/320 kV Nikon Metris $\mu$XCT custom bay shown in Figure 4.2. The specimen and the wedge loading system were placed inside a transparent Perspex tube and the tests were performed using 1.25kN DEBEN loading rig, which was mounted on a rotating stage.
Data were collected at an accelerating voltage of 200kV and 100μA beam current using a tungsten target with a voxel size of 16.9μm. The stage was rotated by 360°, resulting in 2000 2D radiographs for each scan with an angular displacement 0.18°. Each scan took about 30 minutes. To obtain images with a higher resolution, a region of interest located in the middle of the specimens was scanned only (not the whole specimen). Two μXCT in-situ tests were conducted in two days.

The applied load and the vertical displacement readings were recorded by a computer connected with the DEBEN loading rig for the two tests and shown in Figure 4.3. The small points along the loading curves indicate the scanning points during each test. The specimens were first scanned before applying any loads. The load was then applied incrementally at a displacement rate of 0.1mm/min and hold during the scan, then re-applied after each scan finished. The second scans were nearly recorded at the end of linear stage for both specimens. In total, 12 and 10 μXCT scans were obtained for the two specimens at different loads, respectively. During each scan a slight unloading took place due to relaxation, as seen in the curves in Figure 4.3.
The loading responses of both specimens (Figure 4.3) are very similar, indicating the repeatability of the test results. In addition, the crack paths in both fractured specimens deviated away from the vertical notches at nearly the same angle, as shown in Figure 4.4. This can be attributed to the effect of the fibre orientation as explained later in this chapter.

Figure 4.3 Loading history of the in-situ wedge splitting tests and the scanning points.

Figure 4.4 Photographs showing overall failure of the tested UHPFRC specimens under wedge splitting loading.
4.2 Image reconstructing and processing

The 2D radiographs were reconstructed into 3D absorption contrast images using the CT Pro and VG Studio software. Artificial defects such as beam hardening and ring effects were removed by post-processing. The 3D images were then imported into the image processing software AVIZO, and cropped from 2000x2000x2000 (number of slices in $x$, $y$ and $z$ directions respectively) to about 1143x1417x879 to exclude voxels associated with outside air and regions with low contrast. Figure 4.5 shows a 2D slice for the specimen at zero loading before and after cropping respectively. The contrast of the X-ray images was then enhanced by applying filters available in AVIZO. After several trials, it was found that the best contrast can be achieved by applying the median filter and the non-local mean filter to smooth out noise.

![Figure 4.5 X-ray image for the UHPFRC specimen shows the slice before and after cropping.](image)

As shown in Figure 4.5 and 4.6, the highly absorptive steel fibres appear in white, while pores and cracks appear in black, and mortar is uniformly grey reflecting uniform density.
4.2.1 Greyscale-based segmentation

The µXCT images are basically greyscale ones in which voxel values vary on a scale from black to white. Image thresholding was applied to separate/segment the phases according to the greys value of each voxel. The LINE-PROBE command in AVIZO was used to show the greyscale values along a region of interest in a cropped view (Figure 4.7). The region spans across pores, fibres and mortar matrix, in which the greyscale values of the voxels range from 0 to 150. Two lines were drawn in Figure 4.7 to separate the material phases: one at 25 and another at 40, so that all voxels with greyscale values less than 25 are classified as pores, and all voxels with values higher than 40 are considered as the fibre phase, while the voxels with values between 25 and 40 are mortar. These values were chosen based on several considerations and comparisons as explained in the next sections. The LABEL-FIELD function in AVIZO was then used to label the different phases. Further functions such as growing, shrinkage and smoothing were also used to improve the segmented images. The µXCT dataset acquired at zero loading in the first in-situ test was segmented to characterise the UHPFRC specimen's internal structure and presented in the next sections.
Figure 4.7 Greyscale value variation along the path A-B and the thresholding values.

4.3 Material characterisation

4.3.1 Porosity segmentation and analysis

As the pore size covers a wide range (Figure 4.5 and 4.6), a proper selection of greyscale threshold for pores is important. A suitable threshold value was selected such that almost all the pores in the images are covered. A sensitivity study on the threshold selection was carried out. The threshold value was increased from 23 to 28 with an increment of 1, and the respective area picked out on a single 2D slice is shown in Figure 4.8. The variation of the volume fraction of pores with respect to the thresholds is shown in Figure 4.9. There is a sharp change observed in this curve near the threshold value of 26, indicating that a significant volume of the mortar phase is considered as pores for values higher than 26. Hence, a conservative threshold value of 25 was assumed to be sufficient to cover most of the pores without significant inclusion of other phases. Manual corrections were preformed to correct some of the automatically selected pores. Figure 4.10 compares an un-segmented 2D slice with the segmented pores at a threshold value of 25. The measured total volume fraction of the pores for this threshold value is 2.55 %.
Figure 4.8 Pores identified using different greyscale thresholds in a single 2D slice.

Figure 4.9 Sensitivity of pores volume fraction to the greyscale threshold.
CHAPTER FOUR

IN-SITU $\mu$XCT TEST OF UHPFRC

Figure 4.10 Segmented pores covered at a greyscale threshold value of 25.

The 3D network of the segmented pores was reconstructed, and shown in Figure 4.11 with large pores in purple, small pores in green. The notch (in red), which is located in the middle of the segmented volume, is also shown in this figure. It can be seen that most of the pores are nearly spherical in shape.

Figure 4.11 Segmented 3D $\mu$XCT image of pores with large pores in purple, small pores in green and the notch in red.
The volume of each pore was calculated by counting the voxels inside it using a Matlab code. Then, the equivalent diameters \((d_e)\) of individual pores were calculated, assuming each pore is a sphere. The frequency histogram of \(d_e\) was then obtained and shown in Figure 4.12. The total number of segmented pores in this specimen is 10284, and among them 63.3\% has \(d_e=40-300\mu m\), 27.3\% has \(d_e=300-600\mu m\) and 9.4\% has \(d_e=600-1800\mu m\), respectively.

![Frequency distribution of pores’ equivalent diameters.](image)

**Figure 4.12 Frequency distribution of pores’ equivalent diameters.**

### 4.3.2 Fibre segmentation and analysis

A sharp distinction exists between steel fibres and the mortar matrix due to the highly absorptive property of steel fibres, which appear very bright in the X-ray images (Figure 4.6). Thus, a threshold 40 is easily identified for steel fibres so that the average value for the diameter of the fibres matched the known physical diameter of 0.2mm. Some fibres appeared to touch each other (Figure 4.6). Manual separation procedures were used to separate the fibres wherever they appeared to be connected, using the brush tool in AVIZO. Figure 4.13 shows the segmented 3D \(\mu\) XCT image with \(N_f=988\) steel fibres with grey value \(\geq 40\).
The segmented fibres were saved separately as 2D image files and further processed to determine their orientations and locations. First, a skeletonisation algorithm implemented in Matlab developed by Kollmannsberger (Kerschnitzki et al., 2013) was used to identify the centreline of each fibre. Skeletonisation (also known as thinning) is a morphological operation that can be applied on binary images to remove voxels iteratively until only the skeleton of the object is left. This process results in a one voxel-thick fibre skeleton. Then, the orientation angles of each fibre were calculated from the centreline’s coordinates. The orientation of randomly distributed fibres in 3D is commonly characterised by determining two independent angles for each fibre: the in-plane angle ($\theta$) which ranges from 0° to 180° and the out-of-plane angle ($\phi$) which ranges from 0° to 90° (Soroushian and Lee, 1990). The definition of these angles with respect to global axes of the specimen is shown in Figure 4.14c.

The distribution of fibre orientation angles is shown in Figures 4.14a and b. It should be kept in mind that the out-of-plane angle ($\phi$) is the fibre orientation angle that has a significant effect on the fibre pull-out behaviour as explained in section 2.1.2.1 (Li, 1992). The directions of the global axes ($x$, $y$, and $z$) with respect to the notch of the
scanned specimen can be seen in Figure 4.11. The orientation factor defined in equation 3.7 (section 3.3) was calculated with respect to the global axes $x$, $y$, and $z$. It was found that the orientation factor of the fibres with respect to the $x$-axis ($\eta_1 = 0.64$) is higher than the orientation factors with respect to $y$- and $z$- axes ($\eta_2 = 0.30$ and $\eta_3 = 0.56$). These values suggest that the majority of the fibres tend to align along the $x$-axis (the direction of the splitting load).

![Distribution of out-of-plane and in-plane angles](image)

a) Distribution of out-of-plane angles.  
b) Distribution of in-plane angles.

c) Definition of the orientation angles.

Figure 4.14 Distribution of the fibre orientations in 3D.

4.4 Optical microscopy observations at the surface of the specimen
The mortar matrix contains silica sand particles with average diameter 0.27mm (Hassan et al., 2012), as shown in Table 4.1. However, the mortar matrix appears in the $\mu$XCT images uniformly grey reflecting uniform density. Siliceous sand has similar grey level to that of calcium silicate hydrate CSH gel, particularly for dense mortar (Yang & Qin, 2001). The sand particles on the surfaces of the UHPFRC specimen can be seen clearly
using an optical microscopy. Figure 4.15 shows the detailed micro-structure of a small area (2.3×1.8mm) for the mortar matrix, where many sand particles embedded in the cement paste can be seen clearly.

Figure 4.15 Optical microscopy image of mortar matrix.

4.5 Fracture behaviour of the UHPFRC specimen

In this section, the fracture behaviour of the UHPFRC is characterised using the μXCT images acquired for the specimen used in the first in-situ test only (the blue loading curve in Figure 4.3). This particular in-situ test was selected because it has more CT scans than the second one. The scanning points on the load-displacement curve were labelled from 1 to 12 for this in-situ test and re-plotted in Figure 4.16 for clearer explanations.
The initial response of the load-displacement curve is linear corresponding to the elastic stage of the un-cracked specimens. Cracks were observed in the dataset acquired at the second scan (point 2 in the loading history curve shown in Figure 4.16) at which the first deviation from linearity occurred. A very narrow crack (3-5 voxels in width) initiated at the notch and run vertically towards the bottom. The detected crack is illustrated in Figure 4.17 using 2D slices on different planes with cracks highlighted for clear visualisation. The load was increased after this scan nonlinearly up to the peak, at which the third scan was recorded. The nonlinearity in the curve between scan 2 and scan 3 is related to the crack formed in the matrix and arrested by the fibres, leading to dispersed micro-cracks as shown in the X-ray image from scan 3 shown in Figures 4.18 and 4.19. These results suggest that the ultimate load is related to the toughening effects of the fibres (Boulekbache et al., 2015; Mobasher et al., 1990; Shah & Ouyang, 1991).

The post peak response in the loading history tends towards a plateau, indicating stable crack growth. This behaviour is typical in the wedge splitting test, which is commonly described as a very stable fracture test (Karihaloo et al., 2003).
Figure 4.17 µXCT images from scan 2 showing the formed crack at the end of the linear stage.

The micro-crack shown in Figure 4.17 evolved and branched in the subsequent scans during loading, leading to several damage mechanisms, stemming from interactions between cracks and the micro-structure. In the next section, these mechanisms were characterised and discussed at different loading stages.

4.5.1 Characterisation of the damage mechanisms in 2D

Figure 4.18 shows the µXCT images in the xz-plane taken from scans 3 to 11 at the same location. The alignment of the fibre in this slice in the xz-plane allows clearer observation for the interaction between cracks and this fibre. The orientation angle of this fibre with respect to the direction of the horizontal splitting load ($F_1$ in Figure 4.1d) is 23.6° (Figure 4.19). Figure 4.21 shows the location of this slice (as well as other slices used in this section) with respect to the cropped volume.
Figure 4.18 μXCT images in xz-plane showing the evolution of cracks at the same location for scans from 3 to 11.
The μXCT images illustrated in Figure 4.18 show that the cracks initiated from the notch and propagated towards the right support under the specimen. With the increase of applied displacement, some cracks ran upwards (firstly observed in scan 6 shown in Figure 4.18) until they reached the notch at scan 11. The propagation of the cracks towards the notch was observed in several locations at different loading stages. These cracks are related to the wedge splitting test configuration, not to the UHPFRC behaviour.

Figure 4.18 shows the crack arresting mechanism, where the steel fibres restrain the development of matrix cracking. Figure 4.19 shows a magnified view of the intersection between the crack and three fibres labelled from 1 to 3, for four successive scans from 3 to 6. It can be seen that the crack at scan 3 split into several smaller cracks at 1mm ahead of the fibre 1 interface, and these micro-cracks propagated and widened in the subsequent scans. Arresting cracks in a cementitious matrix by reinforcing fibres increases the area of the cracking surfaces in the matrix and thus increases the energy dissipated by the matrix. Trainor et al. (2012) found that about 35%-48% of the total dissipated energy in the fibre reinforced concrete was dissipated through the matrix fracture.

Figure 4.19 Magnified view of the intersection between fibres and cracks for scans 3-6 for the μXCT images shown in Figure 4.18.

Figure 4.18 also shows that the crack path deviates away from its originally vertical orientation (also in Figure 4.4). This can be related to the tendency of the crack to run parallel to the inclined fibres in the weak interfacial zone between the fibres and the surrounding matrix, forming "pseudo-debonding" crack segments (Bentur et al., 1985).
As the orientation angle of a fibre increases, the crack runs for longer distance in the weak interfacial zone before it crosses the fibre. Thus, fibres lying in the plane of the cracks act as a defect that facilitates crack propagation along their interfaces. The propagation of cracks along the fibre-mortar interface was observed in several locations at different loading stages with different "pseudo-debonding" crack segment lengths, for example Figure 4.20. The slices shown in Figure 4.20 located at about 1mm from the slices shown in Figure 4.18 as shown in Figure 4.21.

Figure 4.20 Cracks propagate parallel to the inclined fibre through the weak fibre-matrix interface.
In addition, clear bending of the inclined fibres can be seen in Figure 4.18 and Figure 4.20. The fibre started to bend at two points in scan 4 and the bending level increased in the subsequent scans. It is worth noting that, the fibre started to bend even when the micro-cracks were very narrow. As the loading increases, the fibre segment between the two bending points change its direction and tend to orient horizontally, parallel to the direction of the tensile loading.

Fibre bending was also observed for fibres with short embedment length such as the fibre shown in Figure 4.22. However, if the embedment length is quite short, cracks may rotate around the fibre end instead of crossing it, and thus fibre does not bend. Figure 4.23 shows the arresting mechanism for a crack propagating upwards in a slice taken from scan 7. However, the fibre end in this slice is close to the intersection between the crack and the fibre, thus it turned around the close fibre end (scan 9 and 11). This is because cracks take place where minimum resistance exists (Markovic, 2004).
Turning cracks around fibre ends was observed for cracks running in both upward and downward directions, when the fibre end is close enough to the intersection with the crack. The \(\mu\)XCT image shown in Figure 4.24 shows a crack turns around a fibre end in two successive scans: 4 and 5, and then runs along the fibre interface to some distance. This mechanism should be considered carefully when evaluating the mechanical properties of this material using notched specimens. In real fibre reinforced structures without notches, the cracks are free to search for the weakest zones to propagate through, while in notched specimens cracks are less free to choose its path. Tensile strength values
obtained by testing notched specimens could be higher than those obtained from un-notched specimens (Chanvillard & Rigaud, 2003).

Fibre pull-out was also observed in the µXCT images as the cracks became wider with increasing displacement. Figure 4.25 shows the end slip of a fibre at scans 4, 7 and 10, which increased from 0.1mm at scan 4 to 0.65mm at scan 10.
Figure 4.25 Fibre pull-out mechanism under different loading stages.

Although most of the fibres were pulled out from the shorter embedment length, it was noticed that some fibres pulled out from its longer embedded length. Figure 4.26 shows a 3D isosurface rendering of a fibre with shorter and longer embedment length 4.6mm and 8.4mm respectively. The fibre orientation angle is 32.5°. It can be seen that the slip at the longer side is 0.6mm at scan 10. However, there is no slip at its shorter side. The ability of the fibre to slip from both sides was also reported in the literature by direct measurements of the length of the fibre segments at the fracture surfaces (Markovic, 2006). This phenomenon can be attributed to the effect of the surrounding mortar matrix on the pull-out mechanism (Markovic, 2006). The bond between the fibre and the surrounding matrix at the longer side is weaker than the bond at the shorter side.
The last mechanism observed here is the spalling of the matrix shown in Figure 4.27. In this mechanism, the stress generated by the bending of the fibres at the fibre exit points leads to local damage in the matrix at the crack faces.

4.5.2 Crack surfaces and bridging fibres in 3D

3D visualisation of the crack surfaces is very helpful for understanding the crack morphology. The evolution of matrix cracking is shown in Figure 4.28 for scans 4, 7, 10
and 12 corresponding to the applied displacements 1, 2, 3 and 4mm (Figure 4.16). As the displacement increases, the volume of the cracks increases. The cracks propagated from the notch and inclined in the same direction through its thickness.

The cracks in Figure 4.29 were segmented for a sub-volume cropped from scan 10. Three slices taken from different locations in the sub-volume were also shown in this Figure. The multiple cracking behaviour is clearly visible.
Figure 4.29 Crack surfaces (in green) and bridging fibres (in red) visualisation with views from different locations for a sub-volume from scan 10.

Figure 4.30 shows the same sub-volume in Figure 4.29 but in a transparent view for better visualisation of the bridging fibres. It can be seen that the cracks are bridged with several fibres at different orientation angles. The bending behaviour of inclined fibres can be clearly seen.

Figure 4.30 3D crack surface (in green) and bridging fibres (in red) for the sub-volume shown in Figure 4.29 from two different views.
In Figure 4.31, the cracked matrix and the bridging fibres were illustrated in 3D for another sub-volume in scan 10 from two different views. Here, pores and cracks were considered as empty volumes inside the mortar matrix. This figure illustrates the multiple cracking behaviour in the matrix, and the matrix spalling discussed above. The bridging and bending of the fibres can be also visualised. Moreover, the tendency of the cracks to run parallel to the bridging fibres in the weak fibre-matrix interface can be also seen clearly.

Figure 4.31 3D surfaces for the cracked mortar matrix (in grey) and bridging fibres (in red) for a sub-volume from scan 10 at two different views.

4.5.3 Quantifying the evolution of the cracks

For each slice, the volume fraction of pores and cracks was calculated and plotted along the specimen height (z-axis) in Figure 4.32. The volume fraction of pores and cracks increased with increasing displacement as damage accumulated in the specimen. As expected, the increase is more significant at the top of the specimen. Figure 4.33 shows that the total volume fraction of pores and cracks was steadily increased from 2.55% in the first scan to 12.25% in the last scan, mainly due to matrix cracking and fibre pull-out.
Figure 4.32 The variation in pores and cracks contents along the specimen height during loading.

Figure 4.33 Pores and cracks volume fraction at different scans.

4.6 Effective fibres across the crack
The number of fibres crossing the cracked section in this specimen was 106, corresponding to fibre density 0.442 fibre/mm$^2$. However, not all fibres contributed in the
strength of the specimen as explained above. The effective fibres were assumed to experience bending and pull-out mechanisms. The effective fibre number was counted from different scans by observing its behaviour, and it was about 40 fibres, corresponding to 37.7% of the total fibres.

4.7 Load versus crack width curve

The variation in the crack width under loading was measured from the \( \mu \)XCT images and plotted versus the load. The crack width was measured using the image processing software ImageJ, by computing the increase in the notch width at different loading stages. Several measurements were taken for the notch width, using a slice located at the bottom of the notch shown in Figure 4.34, at locations A to G. The values obtained from the ImageJ represent the number of pixels along the chosen line. These values were multiplied by the pixel size (0.0169mm) to convert it to millimetres. Then, the measured values were averaged and subtracted from the original notch width at scan 1. The load versus the crack width is shown in Figure 4.35.

Figure 4.34 A slice located at the bottom of the notch and the location of points (from A to G) which were used to measure the crack width during loading.
4.8 Summary

The μXCT technique has been used to conduct in-situ wedge splitting tests for the UHPFRC specimens. The procedures for the in-situ test, the reconstruction and segmentation of the μXCT datasets were presented. The μXCT images obtained from the first in-situ test were used to analyse the UHPFRC internal structure and study the cracking mechanisms. The volume fraction of pores in this specimen was 2.55% and its fibres content was 2.57%. The equivalent diameters of the pores range from 40µm to 1800µm. The distribution of the fibre orientations was analysed and the orientation factors with respect to x-, y- and z- axes were 0.64, 0.30 and 0.56 respectively.

The toughening mechanisms at different loading stages were identified, highlighting the interaction between formed cracks and the local micro-structure of the UHPFRC. These mechanisms include arresting of cracks in the matrix by reinforcing fibres, changing of crack direction to align with the weak fibre-matrix interface, bending of inclined fibres, pulling out fibres at either its longer or shorter ends and spalling of mortar at the fibre exit points. Moreover, multiple cracking mechanism and turning of cracks around the close
fibre end were also characterised. 2D images and 3D volumes were both used to describe these mechanisms at different loading stages. The percentage of the number of the effective fibres crossing the crack section was found 37.7%. In addition, the crack width at the notch tip was measured at different loading stages and plotted against the load.
Chapter 5: Image-Based Two-Scale Homogenisation For Elastic Properties of UHPFRC

This chapter presents a two-scale analytical-numerical homogenisation method to predict the effective elastic properties of UHPFRC, considering the distribution of pore sizes in μXCT images of 24.8μm resolution. In the first scale, the mortar, consisting of sand, cement paste and a large number of small pores (equivalent diameter \(d_e=10\sim600\mu m\)), is homogenised using analytical Mori-Tanaka method with constituents' moduli from micro-indentation. In the second scale, the μXCT images of a 20mm cube are converted to mesoscale representation volume elements for finite element homogenisation, with fibres and a small number of large pores (\(d_e=600\sim1400\mu m\)) in the homogenised mortar. The results were compared with experimental data. The effects of model size, fibre volume fraction and fibre orientation on the predicted elastic modulus were investigated.

5.1 μXCT scanning, segmentation and image analysis

5.1.1 Scanning procedures and parameters

A 20mm cube was cut from the same UHPFRC beam, from which the specimens used in the in-situ test were taken (Chapter 4), and scanned at Henry Mosley X-ray Imaging Facility (University of Manchester, UK), using Nikon XTEK XTH 225kV machine with 130 kV and 110μA intensity. The stage was rotated by 360°, resulting in 2985 2D radiographs with an angular displacement of 0.1206° and a voxel resolution of 24.80 μm. The scan took about 17 minutes. The 2D radiographs were then reconstructed into 3D absorption contrast images using the CT Pro and VG Studio software and imported into AVIZO for further processing. The median filter was applied to smooth out noise.

5.1.2 Comparing the μXCT images obtained for the 20mm cube with that obtained for the in-situ test specimens

The μXCT images obtained for the 20mm UHPFRC cube have much better contrast than the μXCT images acquired for the in-situ test specimen (Chapter 4). This can be clearly seen in the slices shown in Figures 5.1a and b. These slices show some black areas (having greyscale value similar to the pores) around some fibres. Automatic segmentation based on greyscale values mistakenly labels these areas as pores, and manual operations were then needed to move these voxels from the air label to the mortar label, which could
reduce the accuracy of the segmented pores. These artefacts are more pronounced in the in-situ test scans than in the 20mm cube scan. This may be due to the higher energy used during the image acquisition (200kV in the in-situ test scans compared with 130kV for 20mm cube scan). Moreover, the use of Perspex tube with the loading rig reduced the contrast of the µXCT images acquired during the in-situ test.

Figure 5.1 Comparing the contrast and the artefacts in µXCT images acquired for the in-situ test specimens with that obtained for the 20mm cube.

5.1.3 Porosity segmentation and analysis

The µXCT data was segmented into different phases according to greyscale thresholds using the software AVIZO. The greyscale values of the µXCT images acquired for the 20mm cube range from 0 to 255. A sensitivity study on the threshold selection was conducted and presented in Figures 5.2 and 5.3. Figure 5.2 shows that the pore volume fraction has a big jump at 60, indicating that some mortar matrix may be mistakenly identified as pores. This is also reflected in the segmented pores shown in Figure 5.3. After careful comparison of the segmented images and the original ones, a threshold 55 was found sufficient to cover most of the pores in all µXCT images. Figure 5.4 compares an un-segmented 2D slice with the segmented one at a threshold value of 55.
Figure 5.2 Sensitivity of pore volume fraction to the greyscale threshold.

Figure 5.3 Pores identified using different greyscale thresholds.
a) Un-segmented µXCT image.  

b) The segmented pores in red.

Figure 5.4 Segmented pores covered at a greyscale threshold value of 55.

Figure 5.5 shows the segmented 3D image of the pores with grey value ≤ 55. Similar to the in-situ test scan, most of the pores in the UHPFRC cube are nearly spherical in shape as shown in Figure 5.5. The resultant pores volume fraction was 2.99% which is slightly higher than the pores volume fraction in the in-situ specimen segmented in Chapter 4 (Figure 4.11). This is due to the enhanced contrast of the µXCT images acquired for the 20mm cube, as explained in the previous section.

Figure 5.5 Segmented 3D µXCT image of pores with large pores in purple and small pores in green.
The frequency histogram of the pores equivalent diameter ($d_e$) was obtained and shown in Figure 5.6. It was found that the total number of pores is 12311, and among them 58.5% has $d_e=25-200\mu$m, 28.3% has $d_e=200-350\mu$m and 13.2% has $d_e=350-1400\mu$m, respectively. In this study, 97.7% of pores with $d_e \leq 600\mu$m were classified as small pores and 2.3% with $d_e=600-1400\mu$m as large pores. The volume fraction for the small pores and the large pores are 1.56% and 1.43% respectively from the image analyses. Smaller pores were captured in these $\mu$XCT dataset than the dataset of the in-situ test specimen because of the better image contrast.

![Frequency distribution of pores’ equivalent diameters.](image)

**Figure 5.6** Frequency distribution of pores’ equivalent diameters.

### 5.1.4 Fibre segmentation and analysis

A threshold 140 was identified for steel fibres with consideration of the fibre diameter 0.2mm. The voxels with grey values between 55 and 140 are then identified as the mortar matrix. The fibres were then separated from one another, wherever they touch each other (Figure 5.1a) using manual separation procedures in AVIZO. Figure 5.7 shows the
segmented 3D µXCT image of \( N_f = 1533 \) number of fibres with grey value \( \geq 140 \). The fibre volume fraction, which equals to 3.75%, is much higher than the 2% used in the mix design (Table 4.1) and the 2.57% identified in the specimen used in the first in-situ test (section 4.3.2), indicating non-uniform distributions of fibres in the UHPFRC beam, from which the specimens were cut. This is a common problem in manufacturing of UHPFRC specimens (Abrishambaf et al., 2013).

![Segmented 3D µXCT image of steel fibres.](image)

Figure 5.7 Segmented 3D µXCT image of steel fibres.

The segmented fibres were saved separately as 2D image files and processed to characterise the overall orientation of fibres using the skeletonisation algorithm (Kerschnitzki et al., 2013) as explained in section 4.3.2. The distribution of out-of-plane (\( \phi \)) and in-plane (\( \theta \)) angles of the random fibres can be shown in Figures 5.8a and b respectively. Figure 5.8c shows the definition of these angles with respect to the global axes. The overall \( \eta_1 \) were then computed with respect to the global axis using equation 3.7. The orientation factor with respect to the \( x \)-axis \( \eta_1 = 0.68 \) is higher than the orientation factors with respect to \( y \)- and \( z \)-axes (\( \eta_2 = 0.42 \) and \( \eta_3 = 0.25 \)), indicating that the majority of fibres in this specimen tend to align along the \( x \)-axis.
5.2 Micro-indentation tests

5.2.1 Specimen preparation

The micro-indentation test was used to measure the elastic moduli of mortar components: silica sand and cement paste shown in Figure 4.15. Specimen used in this test (20x20x10mm³) was cut from the UHPFRC beam and prepared by grinding and polishing its surfaces to obtain reliable and repeatable indentation measurements.

5.2.2 Micro-indentation test

The indentation test is basically based on forcing an indenter into the surface of the material and recording the continuously changing applied load along with the penetration depth. Then, the obtained load-depth curves are used to derive the mechanical properties for the material located directly below and around the indenter.
The micro-indentation tests were carried out using a CSM micro-indentation test machine (CSM, 2010) with Vickers indenter, using different peak forces from 0.3 N to 1.0 N. The indentation machine (shown in Figure 5.9) used in this test is attached to an optical microscopy, with magnifications of 5x and 50x, to help in selecting proper indentation points and to confirm that the indentation has been carried out correctly after the test. The specimen was fixed on a moving table to facilitate its movement between the microscopy and the indenter. The indentation machine can be used to conduct measurements at locations chosen manually by the operator one by one, or it can be assigned to perform a serial of measurements with pre-determined spacing between the indentation points.

Figure 5.9 CSM micro-indentation test machine.

Indentation tests were carried out on different sand particles and cement points. The indentation points were chosen randomly with a sufficient large spacing between them to avoid any interaction between two adjacent indentations. Before starting the indentation measurements, a depth adjustment was first performed using a small contact load. This step is necessary to offset the effect of the deflection of the instrument. Then, the sample was moved a small distance after depth adjustment because a small indentation was performed during this operation as seen in Figure 5.10a, and this could affect the indentation results obtained from the same location. The depth adjustment correction should be repeated for each new location. A total of 150 indentations (65 for cement and
85 for sand) were recorded, processed and stored using the indentation software. Also, the trace of each indent was observed using the attached optical microscopy.

### 5.2.3 Results of the micro-indentation test

Figure 5.10a shows the indentation marks in a sand particle under different peak forces as examples. A row of indentation marks at 0.3N peak force are shown in Figures 5.10b and c in a sand particle and the cement paste, respectively. These indentation marks are clear and have no damaged areas around them, suggesting that they are sufficient to give good estimations of Young’s modulus of the indented area. Figures 5.11 show some examples for load vs. penetration depth curves using 1N peak load.

![Indentation marks in sand and cement](image)

**a)** Indentation in sand using different peak loads.

**b)** Indentation in sand using 0.3N peak load.

**c)** Indentation in cement using 0.3N peak load

Figure 5.10 Indentation marks in sand and cement.
Figure 5.11 Load-depth curves for cement and sand using peak force 1N.

The elastic moduli were calculated from the recorded load-depth curves using Oliver and Pharr method (1992). Figures 5.12a and b show the frequency histogram of the elastic moduli for the silica sand and the cement matrix, respectively. The mean and the standard deviation were 88.61 and 14.46 GPa for the silica sand, compared with 70.00 to 76.30 GPa and 13.00-15.10 GPa for quartz sand in the literature measured by nano-indentation (Da Silva et al., 2014; Sorelli et al., 2008) and micro-indentation (Hemalatha et al., 2014). The obtained mean and standard deviation of elastic moduli for the cement matrix were 58.33 GPa and 14.21 GPa, respectively, compared with much lower elastic moduli for normal cement paste, i.e., 22.80 GPa for water to cement ratio 0.5 (Constantinides & Ulm, 2004).
The interfacial transition zone (ITZ) between the cement paste and the inclusions (sand particles and steel fibres) in UHPFRC differs from that in ordinary concrete and conventional FRC made with higher water to binder ratio (Damidot et al., 2003; Sorelli et al., 2008). The micro-indentation technique is not suitable to test the ITZ in UHPFRC because the thickness of the ITZ is very small (1~5µm) compared with the size of the micro-indentener (>10µm) (Damidot et al., 2003). Figure 5.13 shows indentation marks conducted in this study close to a fibre using the micro-indentation technique. It can be seen that some indentation marks touched the steel fibres, while a few points were indented at the area close to the fibre without touching it, but they are not close enough to be considered representative to the ITZ. Studies from the literature, that tested the ITZ of UHPFRC using a nano-indentation technique, have found that the ITZ is not softer than the bulk cement paste (Damidot et al., 2003; Sorelli et al., 2008). This is because of the enhanced properties of this material due to using low water to binder ratio, eliminating coarse aggregates and using additives such as GGBS and silica fume (Sorelli et al., 2008). Therefore, the ITZ was neglected in the homogenisation method presented in the next sections.
5.3 Two-scale homogenisation method for the UHPFRC

By observing the micro-structures of UHPFRC obtained from the μXCT scanning and the microscopy images (Figure 4.15) and considering the modelling efficiency, a two-scale (referred to hereafter as mortar scale and fibre scale) homogenisation method was developed for predicting the elastic properties of the bulk material as illustrated in Figure 5.14. In the first scale (the mortar scale), the mortar is treated as a three-phase material: sand particles, cement paste and small pores with equivalent diameter less than 600µm. The homogenised elastic properties of the mortar were estimated analytically using the Mori-Tanaka scheme. The elastic properties of the cement paste and silica sand obtained by micro-indentation tests were used as inputs in this scale. In the second scale (the fibre scale), the μXCT images are used to build realistic, finite element models, in which the steel fibres and large pores (having equivalent diameter higher than 600µm) are embedded in the homogenised mortar matrix.

Modelling small pores explicitly in a finite element mesh requires very fine meshes and thus quite expensive FE models will be obtained. Therefore, pores were divided into two groups based on its size: small pores and large pores. Based on the pores size distribution presented in Figure 5.6 (section 5.1.3), it was found a threshold value of 600µm is efficient to separate small pores and large pores, so that only 2.3% of the number of the
observed pores in the µXCT images will be presented explicitly in the finite element meshes in the second scale of homogenisation.

Figure 5.14 Description of the two-scale analytical-numerical homogenisation method for the UHPFRC.

5.3.1 Mortar scale

5.3.1.1 Analytical homogenisation

At the mortar scale, the elastic properties of mortar matrix were predicted using the analytical Mori-Tanaka scheme (Mori & Tanaka, 1973). In this scheme, the homogenised bulk \( k_H \) and shear \( G_H \) moduli of a composite with \( r \) number of inclusion phases can be evaluated using (Da Silva et al., 2014):

\[
k_H = \sum_{c=1}^{r} f_c k_c \left( 1 + \alpha_m \left( \frac{k_c}{k_m} - 1 \right) \right)^{-1} \times \left[ \sum_{c=1}^{r} f_c \left( 1 + \alpha_m \left( \frac{k_c}{k_m} - 1 \right) \right)^{-1} \right]^{-1}
\]

\[
G_H = \sum_{c=1}^{r} f_c G_c \left( 1 + \beta_m \left( \frac{G_c}{G_m} - 1 \right) \right)^{-1} \times \left[ \sum_{c=1}^{r} f_c \left( 1 + \beta_m \left( \frac{G_c}{G_m} - 1 \right) \right)^{-1} \right]^{-1}
\]

with \( \alpha_m \) and \( \beta_m \) defined as:

\[
\alpha_m = \frac{3k_m}{3k_m + 4G_m}
\]
\[ \beta_m = \frac{6k_m + 12G_m}{15k_m + 20G_m} \] (5.4)

where \(k_m\) and \(G_m\) are the bulk and shear moduli of matrix \(m\), and \(k_c\) and \(G_c\) are the bulk and shear moduli of the inclusion \(c (c = 1: r)\) respectively. The parameter \(f_c = \frac{V_c}{V}\) is the volume fraction of the inclusion \(c\) in the volume \(V\), such that \(f_m + \sum_{c=1}^{r} f_c = 1\) and \(f_m\) is the volume fraction of the matrix.

The homogenised bulk and shear moduli are then used to evaluate the homogenised Young's modulus and Poisson's ratio using:

\[ E_H = \frac{9k_H G_H}{3k_H + G_H} \] (5.5)
\[ \nu_H = \frac{3k_H - 2G_H}{6k_H + 2G_H} \] (5.6)

5.3.1.2 Model parameters

At this scale, the mortar is considered as three-phase material in which the silica sand and small pores are inclusions embedded in the cement paste. The analytical model needs the elastic moduli, Poisson's ratios and volume fractions of the involved phases as inputs. The elastic moduli of silica sand and cement paste were taken equal to the mean indentation measurements as \(E_s = 88.61\) GPa, and \(E_m = 58.33\) GPa. The Poisson's ratio is 0.21 and 0.20 for the silica sand and the cement paste respectively (Sorelli et al., 2008).

The volume fractions \(f\) at this level are evaluated based on mass proportions of the mix design shown in Table 4.1. Knowing that the mass density of silica sand is 2652 kg/m\(^3\) (Yang, Millard, et al., 2009), the volume fraction of sand \((f_s)\) calculated from its mass fraction is 39.20%.

The volume fraction of pores \((f_p)\) considered in this model includes large capillary pores and air voids that are resulted from entrapped air with \(d_e > 10\) µm, assuming that the mechanical effects of pores with \(d_e \leq 10\) µm have already been captured by the micro-indentation measurements and thus could be neglected. At the mortar scale, all pores with \(d_e = 10-600\) µm are considered, however the pores smaller than 25µm cannot be identified.
by the µXCT images. The volume fraction of porosity, that are larger than 10 µm, given in the literature for high performance concretes with elastic moduli in the range from 34.9 GPa to 52.7 GPa are between 8.9% and 11.7% (Da Silva et al., 2014; Sorelli et al., 2008). It was found that the relationship between the global elastic modulus of UHPFRC and its porosity up to 10% is approximately linear (Sorelli et al., 2008). Based on this data, the overall porosity \(d_e=10-1400\mu m\) in the scanned UHPFRC specimen with \(E=45.5\) GPa at 28days (Hassan et al., 2012) is assumed to be 10%. As the pores with \(d_e>600\mu m\) modelled at the second scale (fibre scale) has \(f_p=1.43\%\) as revealed in the µXCT scan, the pores modelled at this scale has thus \(f_p=8.57\%\) (10%-1.43%). Finally, the volume fraction of cement at this scale is \(f_m=1-f_p-f_s=1-39.20\%-8.57\%=52.23\%\).

5.3.2 Results of the mortar scale

Table 5.1 summarises the input-output properties of the first scale of homogenisation mortar. The homogenised Young’s modulus of the mortar matrix was 57.30GPa and the Poisson's ratio was 0.207. These values were used to describe the elastic properties of the mortar matrix in the second scale.

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
<th>(E) (GPa)</th>
<th>(v)</th>
<th>(f) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td>Homogenised mortar</td>
<td>57.30</td>
<td>0.207</td>
<td>-</td>
</tr>
<tr>
<td>Cement</td>
<td></td>
<td>58.33</td>
<td>0.20</td>
<td>52.23</td>
</tr>
<tr>
<td>Small pores (d_e\leq600\mu m)</td>
<td></td>
<td>-</td>
<td>-</td>
<td>8.57</td>
</tr>
<tr>
<td></td>
<td></td>
<td>88.61</td>
<td>0.21</td>
<td>39.20</td>
</tr>
</tbody>
</table>

5.3.3 Fibre scale

5.3.3.1 Numerical homogenisation

Numerical homogenisation method was applied at fibre scale to estimate the elastic properties of the UHPFRC (Kanit et al., 2003; Sharma et al., 2013). The average stress and strain can be obtained from the local elemental stresses and strains using the following equation:
\[
\langle \sigma_{ij} \rangle = \frac{1}{V} \left[ \int_{V_m} \sigma_{ij}^m \, dV_m + \int_{V_f} \sigma_{ij}^f \, dV_f \right]
\]  
(5.7)

\[
\langle \varepsilon_{ij} \rangle = \frac{1}{V} \left[ \int_{V_m} \varepsilon_{ij}^m \, dV_m + \int_{V_f} \varepsilon_{ij}^f \, dV_f \right]
\]  
(5.8)

where \( V \) is the volume of the RVE, \( V_m \) and \( V_f \) are the volumes of mortar and fibre phases respectively. However, averaging the local stresses and strains over all elements could be a cumbersome task, especially for RVEs with large number of elements. According to Gauss theorem, the volume average deformation is the same as the deformation of the boundary. Thus, the average stresses and strains can be obtained from the boundaries reaction forces and displacements using (Sun & Vaidya, 1996):

\[
\langle \sigma \rangle = \frac{1}{2|V|} \int_s \left( t_i x_j + t_j x_i \right) ds
\]  
(5.9)

\[
\langle \varepsilon \rangle = \frac{1}{2|V|} \int_s \left( u_i n_j + u_j n_i \right) ds
\]  
(5.10)

where \( s \) is the boundary of the RVE, \( t \) is the traction on the boundaries, \( x \) is the position vector, \( u \) is the displacement and \( n \) is the unit normal vector. The homogenised elastic properties of the UHPFRC can then be evaluated using the generalized Hook's law (equation 2.5) as explained in section 2.4.1.

Two types of boundary conditions were used in this model: periodic boundary conditions (PBC) and kinematic uniform boundary conditions (KUBC). The RVEs were subjected to normal and shear displacements along the three axes of coordinates. In case of PBC, the following loading cases were imposed (Sharma et al., 2013):

Applied normal displacement:

\[
u_x(0,y,z) = u_y(x,0,z) = u_z(x,y,0) = u_y(x,l,z) = u_z(x,y,l) = 0
\]

and \( u_x(l,y,z) = \varepsilon_{11} l \)  
(5.11)

\[
u_x(0,y,z) = u_y(x,0,z) = u_z(x,y,0) = u_x(l,y,z) = u_z(x,y,l) = 0
\]  
(5.12)
and \( u_y(x, l, z) = \varepsilon_{22} l \)

\[
\begin{align*}
    u_x(0, y, z) &= u_y(x, 0, z) = u_z(x, y, 0) = u_x(l, y, z) = u_y(x, l, z) = 0 \\
    \text{and} \quad u_z(x, y, l) &= \varepsilon_{33} l \tag{5.13}
\end{align*}
\]

Applied shear displacement:

\[
\begin{align*}
    u_x(x, 0, z) &= u_y(0, y, z) = u_y(l, y, z) = u_z(0, y, z) = u_z(x, 0, z) = \\
    u_x(x, y, 0) &= u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = 0 \quad \text{and} \quad u_x(x, l, z) = \varepsilon_{12} l \tag{5.14}
\end{align*}
\]

\[
\begin{align*}
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = \\
    u_y(x, y, l) &= u_x(x, y, l) = u_y(x, 0, z) = u_z(0, y, z) = u_z(x, y, l) = \varepsilon_{23} l \\
    \text{where} \ u_x, u_y \text{ and } u_z \text{ are the displacements along the } x-, \ y- \text{ and } z- \text{ axes, respectively, and } l \text{ is the side length of the cubic RVE. The loading cases for KUBC (equation 2.10) can be detailed as follows (Kanit et al., 2003):}
\end{align*}
\]

Applied normal displacement:

\[
\begin{align*}
    u_x(0, y, z) &= u_x(x, 0, z) = u_x(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = \varepsilon_{11} x \\
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_y(l, y, z) = u_y(x, l, z) = u_y(x, y, l) = 0 \\
    u_z(0, y, z) &= u_z(x, 0, z) = u_z(x, y, 0) = u_z(l, y, z) = u_z(x, l, z) = u_z(x, y, l) = 0 \tag{5.15}
\end{align*}
\]

\[
\begin{align*}
    u_x(0, y, z) &= u_x(x, 0, z) = u_x(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = 0 \\
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_y(l, y, z) = u_y(x, l, z) = u_y(x, y, l) = \varepsilon_{22} y \\
    u_z(0, y, z) &= u_z(x, 0, z) = u_z(x, y, 0) = u_z(l, y, z) = u_z(x, l, z) = u_z(x, y, l) = 0 \tag{5.16}
\end{align*}
\]

\[
\begin{align*}
    u_x(0, y, z) &= u_x(x, 0, z) = u_x(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = 0 \\
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_y(l, y, z) = u_y(x, l, z) = u_y(x, y, l) = \varepsilon_{22} y \\
    u_z(0, y, z) &= u_z(x, 0, z) = u_z(x, y, 0) = u_z(l, y, z) = u_z(x, l, z) = u_z(x, y, l) = 0 \tag{5.17}
\end{align*}
\]

\[
\begin{align*}
    u_x(0, y, z) &= u_x(x, 0, z) = u_x(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = 0 \\
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_y(l, y, z) = u_y(x, l, z) = u_y(x, y, l) = \varepsilon_{22} y \\
    u_z(0, y, z) &= u_z(x, 0, z) = u_z(x, y, 0) = u_z(l, y, z) = u_z(x, l, z) = u_z(x, y, l) = 0 \tag{5.18}
\end{align*}
\]

\[
\begin{align*}
    u_x(0, y, z) &= u_x(x, 0, z) = u_x(x, y, 0) = u_x(l, y, z) = u_x(x, l, z) = u_x(x, y, l) = 0 \\
    u_y(0, z, 0) &= u_y(x, 0, z) = u_y(x, y, 0) = u_y(l, y, z) = u_y(x, l, z) = u_y(x, y, l) = 0 \\
    u_z(0, y, z) &= u_z(x, 0, z) = u_z(x, y, 0) = u_z(l, y, z) = u_z(x, l, z) = u_z(x, y, l) = 0 \tag{5.19}
\end{align*}
\]
\( u_z(0,y,z) = u_z(x,0,z) = u_z(x,y,0) = u_z(l,y,z) = u_z(x,l,z) = u_z(x,y,l) = \varepsilon_{33} z \)

Applied shear displacement:

\[
\begin{align*}
\varepsilon_{12} x & = \varepsilon_{12} x (x,y,0) = \varepsilon_{12} x (x,y,z) = \varepsilon_{12} x (x,l,z) = \varepsilon_{12} x (x,y,l) \\
\varepsilon_{23} y & = \varepsilon_{23} y (x,0,z) = \varepsilon_{23} y (x,y,0) = \varepsilon_{23} y (x,y,z) = \varepsilon_{23} y (x,y,l) \\
\varepsilon_{45} z & = \varepsilon_{45} z (0,y,z) = \varepsilon_{45} z (x,0,z) = \varepsilon_{45} z (x,y,0) = \varepsilon_{45} z (x,y,z) = \varepsilon_{45} z (x,y,l) = 0
\end{align*}
\] (5.20)

\[
\begin{align*}
\varepsilon_{13} z & = \varepsilon_{13} z (x,0,z) = \varepsilon_{13} z (x,y,0) = \varepsilon_{13} z (x,y,z) = \varepsilon_{13} z (x,y,l) = 0 \\
\varepsilon_{23} y & = \varepsilon_{23} y (x,0,z) = \varepsilon_{23} y (x,y,0) = \varepsilon_{23} y (x,y,z) = \varepsilon_{23} y (x,y,l) = 0 \\
\varepsilon_{45} z & = \varepsilon_{45} z (0,y,z) = \varepsilon_{45} z (x,0,z) = \varepsilon_{45} z (x,y,0) = \varepsilon_{45} z (x,y,z) = \varepsilon_{45} z (x,y,l) = 0
\end{align*}
\] (5.21) (5.22)

5.3.3.2 Reconstruction of the finite element models

In this scale, the material was modelled using a sequential set of cubic volume elements with increasing lengths: 5mm, 6.5mm, 9mm, 13mm and 16.5mm. To investigate the effects of random distribution of internal phases, a few RVEs at different regions were used for each size: 20 for 5mm, 10 for 6.5mm, 5 for 9mm, 3 for 13mm and 1 for 16.5mm. The RVEs of different sizes are shown in Figure 5.15 with their internal structure (fibres in red and pores in green).

The pores were first sieved from the µXCT images in Matlab to remove small pores \((d_e<600\mu m)\) and then re-combined with fibres and mortar phases, so that the removed small pores were replaced by mortar in the RVEs. Then, the µXCT images were converted into finite element meshes using the commercial software ScanIP (Simpleware Ltd., UK) with element size range \((0.056~0.136mm)\). The mesh for a 5mm cube is shown in Figure 5.16 as an example. It has 213,478 nodes and 902,522 tetrahedron elements (C3D4) for mortar and 231,832 elements for fibres.
Figure 5.15 The volume elements (mortar in blue, fibres in red and pores in green) and the distribution of fibres and pores for RVEs with different sizes.

Figure 5.16 The finite element mesh for 5 mm RVE (fibres in red, and empty pores).
The fibre and the matrix were both considered linear and isotropic in this analysis. The elastic modulus of the steel fibres used in the model was 200GPa and the Poisson’s ratio was 0.3. The Young’s modulus of the homogenised mortar (57.30GPa) and its Poisson’s ratio (0.207) predicted in the first scale of homogenisation were used as basic inputs in the simulations of these volume elements. All the finite element analyses were conducted using ABAQUS version 6.12.

5.3.4 Results of fibre scale

Each FE model was simulated under the loading conditions given in equations 5.11-5.16 using PBC and in equations 5.17-5.22 using KUBC. Figure 5.17 shows the deformation modes with stress contours of a 9mm RVE subjected to KUBC as an example. Figures 5.17 a, b and c show the normal stress contours $S_{11}$, $S_{22}$, and $S_{33}$ (in MPa) under unit normal strain $\varepsilon_{11}$, $\varepsilon_{22}$ and $\varepsilon_{33}$ respectively, while Figures 5.17 d, e and f show the shear stress contours $S_{12}$, $S_{13}$ and $S_{23}$ under unit shear strain $\varepsilon_{12}$, $\varepsilon_{13}$ and $\varepsilon_{23}$ respectively. It can be seen that, the local stresses in the mortar matrix concentrate mainly around pores as well as near the fibre elements. The stresses in the fibres are higher than those in the cement for all loading conditions because they are much stiffer.

Figure 5.17 Stress contours under six loading cases for 9mm RVE using KUBC.
The homogenised stiffness coefficients can be determined using equations 2.5 and 5.7-5.8, and of the first 9mm RVE are shown in equation 5.23. The coupling terms show that extension-shear and shear-shear components were much lower than those of extension-extension and were negligible.

\[
C^H_{ijkl} = \begin{bmatrix}
65.56 & 16.53 & 16.49 & 0.08 & 0.09 & 0.17 \\
64.86 & 16.31 & 0.05 & -0.01 & 0.23 \\
65.36 & -0.02 & 0.10 & 0.32 \\
Symmetric & 24.29 & 0.30 & 0.02 \\
Shear-Shear & 24.17 & 0.01 \\
& & 24.08 \\
\end{bmatrix}
\]  

(5.23)

The calculated means and standard deviations for the five 9mm RVE are:

\[
C^H_{ijkl} = \begin{bmatrix}
65.58 \pm 0.27 & 16.60 \pm 0.13 & 16.45 \pm 0.11 & 0 & 0 & 0 \\
65.58 \pm 0.50 & 16.33 \pm 0.10 & 0 & 0 & 0 \\
64.40 \pm 0.30 & 0 & 0 & 0 \\
Symmetric & 24.32 \pm 0.15 & 0 & 0 \\
& & 24.17 \pm 0.11 \\
& & & 24.08 \pm 0.12 \\
\end{bmatrix}
\]  

(5.24)

The elastic constants were calculated from equation 2.7 and 5.24 for all the RVE sizes under KUBC and PBC and listed in Table 5.2 and 5.3 respectively, where the effective homogenised properties (EHP) are the volume averaged values of all the RVEs. It can be seen that the elastic moduli \(E_{22}\) and \(E_{33}\) are slightly less than \(E_{11}\) for all sizes. This can be related to the orientations of fibres which tend to align with the \(x\)-axis as explained in section 5.1.4.
Table 5.2 Engineering constants of RVEs reinforced by 3D fibre elements with associated uncertainties using KUBC.

<table>
<thead>
<tr>
<th>RVE size (mm)</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$E_{33}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
<th>$\nu_{12}$</th>
<th>$\nu_{13}$</th>
<th>$\nu_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>58.93 ± 1.26</td>
<td>58.34 ± 1.15</td>
<td>57.96 ± 1.34</td>
<td>24.38 ± 0.64</td>
<td>24.21 ± 0.6</td>
<td>24.11 ± 0.6</td>
<td>0.211 ± 0.0019</td>
<td>0.209 ± 0.0019</td>
<td>0.207 ± 0.0017</td>
</tr>
<tr>
<td>6.5</td>
<td>58.67 ± 1.05</td>
<td>58.59 ± 0.78</td>
<td>57.79 ± 0.91</td>
<td>24.28 ± 0.48</td>
<td>24.12 ± 0.39</td>
<td>24.05 ± 0.39</td>
<td>0.210 ± 0.0019</td>
<td>0.207 ± 0.0016</td>
<td>0.208 ± 0.0015</td>
</tr>
<tr>
<td>9</td>
<td>58.83 ± 0.22</td>
<td>58.15 ± 0.44</td>
<td>57.83 ± 0.26</td>
<td>24.31 ± 0.15</td>
<td>24.17 ± 0.12</td>
<td>24.08 ± 0.12</td>
<td>0.211 ± 0.0018</td>
<td>0.210 ± 0.0019</td>
<td>0.210 ± 0.0017</td>
</tr>
<tr>
<td>13</td>
<td>59.11 ± 0.09</td>
<td>58.16 ± 0.41</td>
<td>57.49 ± 0.05</td>
<td>24.21 ± 0.08</td>
<td>24.01 ± 0.03</td>
<td>24.12 ± 0.02</td>
<td>0.212 ± 0.0018</td>
<td>0.209 ± 0.0013</td>
<td>0.209 ± 0.0015</td>
</tr>
<tr>
<td>16.5</td>
<td>59.83 ± 0.32</td>
<td>57.32 ± 0.41</td>
<td>57.57 ± 0.05</td>
<td>24.26 ± 0.06</td>
<td>23.99 ± 0.10</td>
<td>23.85 ± 0.11</td>
<td>0.208 ± 0.001</td>
<td>0.210 ± 0.001</td>
<td>0.208 ± 0.001</td>
</tr>
<tr>
<td>EHP</td>
<td>58.97 ± 0.24</td>
<td>58.10 ± 0.55</td>
<td>57.72 ± 0.19</td>
<td>24.29 ± 0.10</td>
<td>24.10 ± 0.10</td>
<td>24.04 ± 0.11</td>
<td>0.210 ± 0.001</td>
<td>0.209 ± 0.001</td>
<td>0.208 ± 0.001</td>
</tr>
<tr>
<td>Finally averaged</td>
<td>58.26 ± 0.64</td>
<td></td>
<td></td>
<td>24.14 ± 0.13</td>
<td></td>
<td></td>
<td>0.209 ± 0.001</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 5.3 Engineering constants of RVEs reinforced by 3D fibre elements with associated uncertainties using PBC.

<table>
<thead>
<tr>
<th>RVE size(mm)</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$E_{33}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
<th>$\nu_{12}$</th>
<th>$\nu_{13}$</th>
<th>$\nu_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>59.15±1.12</td>
<td>58.18±1.13</td>
<td>58.14±0.98</td>
<td>24.50±0.43</td>
<td>24.36±0.46</td>
<td>24.27±0.41</td>
<td>0.211</td>
<td>0.209</td>
<td>0.207</td>
</tr>
<tr>
<td>6.5</td>
<td>58.83±0.96</td>
<td>58.51±0.88</td>
<td>57.87±0.74</td>
<td>24.38±0.33</td>
<td>24.24±0.39</td>
<td>24.15±0.33</td>
<td>0.211</td>
<td>0.207</td>
<td>0.208</td>
</tr>
<tr>
<td>9</td>
<td>58.83±0.22</td>
<td>59.01±0.41</td>
<td>57.89±0.23</td>
<td>24.10±0.13</td>
<td>24.27±0.11</td>
<td>24.18±0.11</td>
<td>0.210</td>
<td>0.210</td>
<td>0.210</td>
</tr>
<tr>
<td>13</td>
<td>59.13±0.35</td>
<td>58.12±0.59</td>
<td>57.71±0.21</td>
<td>24.20±0.16</td>
<td>24.15±0.64</td>
<td>24.17±0.07</td>
<td>0.211</td>
<td>0.209</td>
<td>0.209</td>
</tr>
<tr>
<td>16.5</td>
<td>58.63</td>
<td>58.61</td>
<td>57.66</td>
<td>24.11</td>
<td>23.96</td>
<td>23.99</td>
<td>0.209</td>
<td>0.210</td>
<td>0.208</td>
</tr>
<tr>
<td>EHP</td>
<td>58.91±0.22</td>
<td>58.48±0.35</td>
<td>57.85±0.19</td>
<td>24.26±0.18</td>
<td>24.20±0.15</td>
<td>24.15±0.10</td>
<td>0.210</td>
<td>0.209</td>
<td>0.208</td>
</tr>
<tr>
<td>Finally averaged</td>
<td>58.42±0.53</td>
<td>24.20±0.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.209</td>
<td>0.209</td>
<td>0.208</td>
</tr>
</tbody>
</table>
The anisotropy ratio \( \alpha \) of the planes was computed for all RVEs using:

\[
a = \frac{2C_{44}}{C_{11} - C_{12}}
\]

(5.25)

where \( C_{11} \), \( C_{12} \) and \( C_{44} \) are coefficients of the homogenised stiffness matrix (equation 2.5) averaged over all RVEs of the same sizes. The anisotropy ratio's were found very close to 1. They were in the range of 0.965-1.013 for both KUBC and PBC, suggesting that the UHPFRC specimen can be considered as isotropic. As a result, the engineering constants can be reduced to isotropic homogenised elastic modulus \( (E) \), homogenised shear modulus \( (G) \) and Poisson's ratio \( (\nu) \) using the following equations:

\[
E = \frac{E_{11} + E_{22} + E_{33}}{3}
\]

\[
G = \frac{G_{12} + G_{13} + G_{23}}{3}
\]

(5.26)

\[
\nu = \frac{\nu_{12} + \nu_{13} + \nu_{23}}{3}
\]

The final homogenised Young’s modulus, shear modulus and Poisson’s ratio are calculated by averaging the three EHP as 58.26±0.64GPa, 24.14±0.13GPa and 0.209±0.001, respectively for RVEs subjected KUBC (also shown in Table 5.2) and 58.42±0.53, 24.20±0.05 and 0.209±0.001 respectively for RVEs under PBC (Table 5.3).

5.3.4.1 Effect of boundary condition

Figure 5.18 plots the RVE size versus the homogenised Young's moduli (averaged by the number of RVEs for each size) and the errors for both PBC and KUBC. This figure shows that the predicted elastic properties of the UHPFRC do not depend on the type of the prescribed boundary conditions. Also, it can be concluded that the 9mm RVE is big enough to yield a stable elastic modulus.
5.3.4.2 Comparison with experimental data and re-modelling

Table 5.4 compares the homogenised elastic moduli $E_H$ of the mortar and the UHPFRC with the experimental data, where $E_e$ is obtained from cylindrical compressive tests (Hassan et al., 2012), $E_u$ from ultrasonic pulse velocity tests and $E_r$ from resonant frequency tests (Hassan & Jones, 2012), all at 28 days. The differences between the homogenised results and the experimental data are shown in the brackets. It can be seen that the homogenised $E_H=57.3\text{GPa}$ for the mortar overestimates the experimental $E_e=42.08\text{GPa}$ by 36.2%, which in turn leads to 13.6~27.9% overestimations for the bulk of UHPFRC. Part of the difference between $E_H$ and $E_e$ in the first scale is due to excluding the big pores with $d_e>600\mu\text{m}$ from this scale. However, the more pronounced reason may be the uncertainties involved in the indentation measurements that are reflected by a relatively high standard deviation in the moduli for the cement paste and the silica sand. Nano-indentation test can be carried out for more accurate results (Da Silva et al., 2014)
Table 5.4 Comparison of homogenised and experimental moduli using the mean values of micro-indentation measurements.

<table>
<thead>
<tr>
<th></th>
<th>$E_H$ (GPa)</th>
<th>$E_e$ (GPa)</th>
<th>$E_u$ (GPa)</th>
<th>$E_r$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar</td>
<td>57.30</td>
<td>42.08 (36.2%)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>UHPFRC</td>
<td>58.26</td>
<td>45.55 (27.9%)</td>
<td>48.25 (20.8%)</td>
<td>51.3 (13.6%)</td>
</tr>
</tbody>
</table>

To clarify this issue, the lower bounds of the indentation results (computed by subtracting the standard deviations from the mean values), $E_{s} = 74.61$ GPa for the silica sand and $E_{cm} = 44.33$ GPa for the cement paste, were used as inputs in the first scale. The homogenised elastic modulus of mortar matrix is 47.17 GPa. This value was then used as input for the 9mm RVEs to be re-modelled, leading to $E_H = 48.23 \pm 0.59$ for the UHPFRC. The resultant differences with the experimental data now become very small as seen in Table 5.5.

Table 5.5 Comparison of homogenised and experimental moduli using the lower bounds of micro-indentation measurements.

<table>
<thead>
<tr>
<th></th>
<th>$E_H$ (GPa)</th>
<th>$E_e$ (GPa)</th>
<th>$E_u$ (GPa)</th>
<th>$E_r$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortar</td>
<td>47.17</td>
<td>42.08 (11.56%)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>UHPFRC</td>
<td>48.23</td>
<td>45.55 (5.88%)</td>
<td>48.25 (-0.04%)</td>
<td>51.3 (-5.98%)</td>
</tr>
</tbody>
</table>

5.3.4.3 Models with 1D fibres

The steel fibres were also modelled by 1D two-noded truss elements to save computational cost so that fast simulations can be carried out for parametric studies. The voxels of fibres in the μXCT images were replaced by mortar. The centrelines for all fibres, obtained from the skeletonisation process aforementioned, were used to generate 1D truss elements (T2D3) (defined by two end-nodes in the global coordinates) using a Matlab code. They were then embedded into the homogenised mortar matrix with perfect bond. Figure 5.19 shows the same RVEs in Figure 5.15 and the distributions of 1D fibres in each RVE. Modelling fibres as 1D lead to considerable reduction in the degrees of freedom in the FE models. For example, using the same element size range (0.056–0.136mm) in the commercial software ScanIP (Simpleware Ltd, UK) as in Figure
5.19, the FE model using 1D truss elements for the 5mm RVE has only 79,131 nodes and 388,195 elements in total, with only 64 truss elements for fibres. All RVEs with 1D fibre elements were analysed using KUBC (equations 5.17-5.22).

![RVE models](image)

Figure 5.19 The RVEs sizes (mortar in blue and pores in green) and the distributions of 1D fibres.

For these models, the homogenised stiffness coefficients were determined from the reaction forces of the RVE boundaries according to the equations 5.9-5.10. The results are shown in Table 5.6. The anisotropy ratios for the all RVEs (equation 5.25) were found in the range of 0.971-0.986, indicating isotropic material behaviour, and hence the homogenised elastic properties can be calculated according to equations 5.26.
Table 5.6 Engineering constants of RVEs reinforced by 1D fibre elements with associated uncertainties using KUBC.

<table>
<thead>
<tr>
<th>RVE size (mm)</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$E_{33}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
<th>$\nu_{12}$</th>
<th>$\nu_{13}$</th>
<th>$\nu_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>58.38 ±1.29</td>
<td>56.84 ±1.21</td>
<td>56.11 ±1.13</td>
<td>24.08 ±0.53</td>
<td>23.61 ±0.65</td>
<td>23.38 ±0.51</td>
<td>0.211 ±0.0019</td>
<td>0.209 ±0.0019</td>
<td>0.207 ±0.0017</td>
</tr>
<tr>
<td>6.5</td>
<td>58.29 ±1.12</td>
<td>56.99 ±0.72</td>
<td>56.14 ±0.67</td>
<td>24.11 ±0.34</td>
<td>23.54 ±0.47</td>
<td>23.41 ±0.32</td>
<td>0.211 ±0.0019</td>
<td>0.207 ±0.0016</td>
<td>0.208 ±0.0015</td>
</tr>
<tr>
<td>9</td>
<td>58.65 ±0.48</td>
<td>56.77 ±0.74</td>
<td>56.58 ±0.27</td>
<td>24.12 ±0.27</td>
<td>23.65 ±0.18</td>
<td>23.45 ±0.11</td>
<td>0.210 ±0.0018</td>
<td>0.210 ±0.0019</td>
<td>0.210 ±0.0017</td>
</tr>
<tr>
<td>13</td>
<td>58.30 ±0.31</td>
<td>56.86 ±0.61</td>
<td>56.60 ±0.12</td>
<td>24.11 ±0.07</td>
<td>23.46 ±0.19</td>
<td>23.31 ±0.08</td>
<td>0.211 ±0.0018</td>
<td>0.209 ±0.0013</td>
<td>0.209 ±0.0015</td>
</tr>
<tr>
<td>16.5</td>
<td>58.62</td>
<td>57.32</td>
<td>55.99</td>
<td>24.17</td>
<td>23.56</td>
<td>23.39</td>
<td>0.209</td>
<td>0.210</td>
<td>0.208</td>
</tr>
<tr>
<td>20</td>
<td>58.59</td>
<td>57.35</td>
<td>55.98</td>
<td>24.14</td>
<td>23.47</td>
<td>23.39</td>
<td>0.211</td>
<td>0.210</td>
<td>0.207</td>
</tr>
<tr>
<td>EHP</td>
<td>58.46 ±0.16</td>
<td>56.93 ±0.39</td>
<td>56.18 ±0.23</td>
<td>24.12 ±0.03</td>
<td>23.55 ±0.07</td>
<td>23.39 ±0.04</td>
<td>0.211 ±0.0008</td>
<td>0.209 ±0.001</td>
<td>0.208 ±0.001</td>
</tr>
<tr>
<td>Finally averaged</td>
<td>57.20±1.16</td>
<td></td>
<td>23.68±0.38</td>
<td></td>
<td></td>
<td></td>
<td>0.209±0.001</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
5.3.4.4 Comparison between RVE models with 3D and 1D fibres

Figure 5.20 plots the RVE size versus the homogenised elastic moduli (averaged by the number of RVEs for each size) and the errors for both 1D and 3D modelling of fibres. From these results, it can be concluded that 9mm is big enough to yield stable elastic modulus for both models, and thus can be regarded as representative. It can also be seen that modelling fibres using 3D or 1D elements made little difference to the homogenised modulus. For example, the homogenised moduli of 9mm model are 58.22GPa and 57.33GPa from 3D and 1D modelling respectively, compared with 57.30GPa for mortar (with small pores only). This is because the effect of fibres in strengthening the matrix is contradicted by the effect of big pores which soften it.

![Figure 5.20 Size effect of RVE models on the predicted homogenised elastic modulus of UHPFRC.](image-url)

Figures 5.21a and b show the distribution of \( S_{11} \) in the fibre elements for the first 9mm RVE with 3D and 1D fibres respectively, subjected to normal loading in the direction of the \( x \)-axis (equation 5.13). It is worth noting that 1D truss elements in ABAQUS have only one stress component which is \( S_{11} \), and it is in the direction of its local axis. Each fibre hold only one constant \( S_{11} \) value, while in 3D fibre elements, the stress \( S_{11} \) distributes along the whole fibre and it is in the direction of the global \( x \)-axis. Figure 5.21 shows the significant effect of the orientation angle of each fibre with respect to the direction of the applied load on the stress held by the fibre in both models. Fibres with
smaller angles have high stress values, and these values decrease with increasing the fibre orientation angle with respect to the direction of the applied load.

It can be seen in Table 5.6 that the values of $E_{22}$ and $E_{33}$ for RVEs with 1D fibres are less than the homogenised elastic modulus of the mortar matrix that was used as input in this scale, while $E_{11}$ is higher. Compared with engineering constants of RVE's with 3D fibre modelling shown in Table 5.4 and 5.5, it can be concluded that modelling fibres as 1D elements has little effect on the stiffness of the RVE's in the $y$ and $z$ directions. This is due to the effect of fibre orientations which become more significant when modelling fibres as 1D truss elements, leading to larger error bars than RVE's with 3D fibres as shown in Figure 5.20. $E_{22}$ and $E_{33}$ in Table 5.6 are less than the homogenised elastic modulus of the mortar matrix because of the softening effect of large pores.

Figure 5.21 Distribution of S11 in the fibres under normal loading in the direction of the $x$-axis for the first 9mm RVE.

5.4 The effect of fibre content on $E$

As the usage of high-strength steel fibres is one of the main reasons for high cost of UHPFRC, the effects of fibre volume fraction were investigated. The 9mm RVE models with 1D fibre elements were re-simulated with $f_r=6\%$, 8\% and 10\% in addition to the original 3.75\%. The X-ray image-based meshes for the mortar with large pores were kept the same for all the models. A Matlab code was developed to randomly add more two-noded fibre elements until the desired volume fraction was reached (Figure 5.22).
eliminate the effect of the fibre orientation, the newly added fibres had the same orientation factors with respect to the global axes as in the original models.

Figure 5.22 Different fibre volume fractions modelled in 9mm RVE modelled.

Table 5.7 shows the engineering constants averaged over the five 9mm RVEs for different fibre volume fraction. The predicted $E_{11}$ are 60.11, 61.33, and 62.27GPa for $f_f=6\%$, 8\% and 10\%, respectively, compared with $E_{11} = 58.65$GPa for $f_f=3.75\%$ from Table 5.6. $E_{22}$ and $E_{33}$ are increased slightly with the increase of the fibre content, as well as the shear moduli. The anisotropy ratio is about 0.98 for the three different fibre content, reflecting isotropic material behaviour. It can be seen that the elastic properties of the UHPFRC are improved with increasing the fibre contents. However, this improvement is limited within about 10\%. Similar results have been found experimentally in the literature (Al-Ameeri, 2013; Prashant et al., 2011; Thomas & Ramaswamy, 2009).

Table 5.7 Engineering constants of 9mm RVE with different fibre contents.

<table>
<thead>
<tr>
<th>$f_f$</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$E_{33}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6%</td>
<td>60.11±0.47</td>
<td>57.32±0.70</td>
<td>56.36±0.27</td>
<td>24.66±0.18</td>
<td>23.94±0.17</td>
<td>23.59±0.09</td>
</tr>
<tr>
<td>8%</td>
<td>61.33±0.71</td>
<td>57.75±0.69</td>
<td>56.42±0.26</td>
<td>25.16±0.22</td>
<td>24.18±0.17</td>
<td>23.71±0.07</td>
</tr>
<tr>
<td>10%</td>
<td>62.27±0.64</td>
<td>58.19±0.75</td>
<td>56.49±0.25</td>
<td>25.58±0.22</td>
<td>24.39±0.17</td>
<td>23.82±0.07</td>
</tr>
</tbody>
</table>

5.5 The effect of fibre orientation on $E$

The five 9mm RVE models with 1D fibre elements and fibre volume fraction of 10\% were then re-simulated to study the effect of fibre orientation on the predicted $E_H$. All
fibres were aligned with the $x$-axis but placed randomly, so the fibre orientation factor $\eta_1$ with respect to $x$-axis is 1 and close to zero with respect to other axes. The averaged elastic moduli are $E_{11}=75.77\text{GPa}$, $E_{22}=56.57\text{GPa}$ and $E_{33}=56.56\text{GPa}$, with little deviations. It can be seen that $E_{11}$ is about 33.94% higher than $E_{22}$ and $E_{33}$ with anisotropy ratio for the five 9mm RVEs is about 0.70, suggesting that the material is no longer isotropic. The modulus in the fibre direction $E_{11}=75.77\text{GPa}$ is about 21.7% higher than $E_{11}=62.27\text{GPa}$ of the 9mm RVE models with same fibre content but randomly oriented. This shows the significant effect of the fibre orientation on the elastic modulus of UHPFRC. The improvement of the elastic properties of UHPFRC with increasing the fibre orientation factor was also shown by Kang & Kim (2011).

5.6 Summary

This chapter has presented an efficient two-scale analytical-numerical homogenisation method to predict the effective elastic properties of the UHPFRC. A 20mm UHPFRC cube was scanned using the $\mu$XCT technique and its micro-structure was analysed using the obtained $\mu$XCT images of 24.8$\mu$m resolution. It was found in the specimen, there are over 12300 pores with size ranging from 25$\mu$m to 1400$\mu$m, among which 97.7% are smaller than 600$\mu$m. Based on the distribution of pore sizes, a two-scale homogenisation approach was developed. In the first scale, the mortar is treated as a three-phase material: sand particles, cement paste and the small pores (with equivalent diameter $d_e<600\mu$m). The homogenised elastic properties of the mortar was estimated analytically using the Mori-Tanaka model. The elastic properties of the sand particles and cement paste were measured using the micro-indentation technique, and the mean values were used as input in the first scale. In the second scale, the 3D $\mu$XCT images were used to build realistic finite element models of RVEs, in which the steel fibres and larger pores (with $d_e>600\mu$m) are embedded in the homogenised mortar from the first scale. Fibres were modelled as 1D two-noded elements and 3D solid elements.

It was found that the 9mm RVE is big enough to yield stable elastic modulus of both models with 1D and 3D fibres, with homogenised elastic modulus of 57.33GPa and 58.22GPa respectively. These values were compared with experimental data, and it was seen that the homogenised elastic modulus of mortar overestimated the experimental
elastic modulus by 36.17%, which in turn led to 13.6~27.9% overestimations for the bulk of UHPFRC. This difference may be related to the uncertainties involved in the micro-indentation tests. The 9mm RVE models were re-simulated using the lower bounds of the indentation measurements, and the differences between $E_H$ and experimental data were reduced considerably. The effects of fibre content and orientations on the $E_H$ were investigated, demonstrating that this method can be used to optimise the material's microstructure. It was found that increasing the fibre content led to a slight increase in the predicted $E_H$. However, aligning fibres in one direction led to larger differences between elastic moduli in different directions, suggesting that the UHPFRC is no longer isotropic material. $E_{11}$ for 9mm RVE with 10% aligned fibres in the direction of the $x$-axis is 21.70% higher than $E_{11}$ for the same fibre content but with randomly distributed.
Chapter 6: Modelling and Validation of In-Situ μXCT Wedge Splitting Test Model

In this chapter, nonlinear finite element models were developed in ABAQUS to simulate the in-situ μXCT wedge splitting test presented in Chapter 4. The centrelines of fibres, obtained from the skeletonisation process, were used to generate 1D two-noded elements in a Matlab code with actual positions and orientations in the tested UHPFRC specimen. They were then embedded into the mortar mesh with perfect bond. The pull-out behaviour of the fibres was modelled indirectly using the constitutive behaviour of the embedded fibres. Concrete damage plasticity model was adopted to simulate the fracture behaviour of the mortar matrix. The numerical results were compared with the in-situ wedge splitting test results.

6.1 Modelling of mortar

The fracture behaviour of the mortar was modelled by the concrete damage plasticity model (CDPM) in ABAQUS. CDPM is intended primarily for the analysis of plain or reinforced concrete subjected to monotonic or cyclic loading under low confining pressure. It uses the concept of isotropic damaged elasticity in combination with isotropic tensile and compressive plasticity to represent the inelasticity and fracture behaviour of concrete. The experimental data obtained from unreinforced mortar specimens (Hassan et al., 2012) were used to define the constitutive behaviour of mortar in compression and tensions, shown in Figure 6.1.
The CDPM was defined in ABAQUS using the keyword *CONCRETE DAMAGE PLASTICITY. The compressive behaviour was implemented using the keyword *COMPRESSION HARDENING, TYPE=STRAIN. The following equation proposed by Saenz (1964) was used to define the stress-strain relationship in Figure 6.1a:

\[
\sigma_c = \frac{E \varepsilon_c}{1 + \left(\frac{E \varepsilon_{cu}}{\sigma_{cu}} - 2\right) \left(\frac{\varepsilon_c}{\varepsilon_{cu}}\right) + \left(\frac{\varepsilon_c}{\varepsilon_{cu}}\right)^2}
\]

(6.1)

where \(\sigma_c\) and \(\varepsilon_c\) are the compressive stress and strain respectively, \(\sigma_{cu}\) and \(\varepsilon_{cu}\) are the experimentally determined maximum stress and corresponding strain, and \(E\) is the elastic modulus of the mortar matrix.

The tensile response of mortar (Figure 6.1b) was defined using the tension softening relationship proposed by Hordijk (1991), which was implemented as a traction-crack opening displacement curve to avoid mesh-dependent results (Chen et al., 2015; Mahmud et al., 2013). This relationship is defined as:

\[
\frac{\sigma_t}{\sigma_{tu}} = \left[1 + \left(c_1 \frac{W_t}{W_{cr}}\right)^3\right] e^{-c_2 \frac{W_t}{W_{cr}}} - \frac{W_t}{W_{cr}} (1 + c_1^3) e^{-c_2}
\]

(6.2)
\[ w_{cr} = 5.14 \frac{G_F}{\sigma_{tu}} \]  (6.3)

where \( w_c \) is the crack opening displacement, \( w_{cr} \) is the crack opening displacement at the complete release of tensile stress, \( \sigma_t \) is the tensile stress normal to the crack direction, \( \sigma_{tu} \) is the ultimate tensile strength of the mortar and \( c_1 = 3.0 \) and \( c_2 = 6.93 \) are constants determined from tensile tests of concrete (Hordijk, 1991). This was implemented in ABAQUS using the keyword *CONCRETE TENSION STEFFENING, TYPE=DISPLACEMENT.

Damage is characterised in CDPM by the stiffness degradation (Figure 6.1), which is defined in ABAQUS by specifying the tensile damage index \( (d_t) \) and the compressive damage index \( (d_c) \). These damage indices vary from 0 for undamaged to 1 for completely damaged material. The tensile damage index \( d_t \) was calculated by (Lubliner et al., 1989):

\[ d_t = \frac{\sigma_{tu} - \sigma_t}{\sigma_{tu}} \]  (6.4)

And the compressive damage index \( d_c \) was computed by:

\[ d_c = \frac{\sigma_{cu} - \sigma_c}{\sigma_{cu}} \]  (6.5)

Equations (6.4) and (6.5) were implemented in ABAQUS using the keyword: *CONCRETE TENSION DAMAGE, TYPE =DISPLACEMENT and *CONCRETE COMPREISSON DAMAGE, TYPE =STRAIN, respectively.

The default values in ABAQUS are used for other material parameters required to determine the flow rule and yield surface, including: dilation angle (36°), flow potential eccentricity (0.1), ratio of initial equi-biaxial compressive yield stress to initial uni-axial compressive yield stress (1.16), ratio of the second stress invariant on the tensile meridian to that on the compressive meridian is equal to (0.6667) and viscosity parameter (0).

**6.2 Modelling of fibres**

Steel fibres were modelled as 1D truss elements using the data extracted from the \( \mu \)XCT images of the in-situ test specimen by the skeletonisation technique. The bond behaviour was defined indirectly by the constitutive model of steel fibres proposed by Cunha et al.
(2011; 2012) and Soetens et al. (2012). In this model, the 1D fibres were perfectly bonded with the mortar mesh. The pull-out behaviour of fibres was calculated analytically using the analytical pull-out model proposed by Naaman et al. (1991) and Lee et al. (2010) as presented in Chapter 3 (section 3.2.3). The obtained pull-out load versus slip \((P - \Delta)\) relationships were then transformed to tensile stress-strain \((\sigma_f - \varepsilon_f)\) relationship and used to represent the constitutive laws of the embedded steel fibres. Figure 6.2 shows the procedures adopted to obtain \((\sigma_f - \varepsilon_f)\) curves. \(\sigma_f\) is calculated as the ratio between the pull-out force and the cross-sectional area of the fibre, while the corresponding \(\varepsilon_f\) is calculated by dividing slip value by the fibre length.

![Figure 6.2 Transformation fibre pull-out curve to equivalent stress-strain relationship (Cunha et al., 2012).](image)

The effects of orientation angle and embedded length of each fibre were considered. To simplify modelling, the fibres were divided into five groups according to their orientation angles \([0^\circ-15^\circ], [15^\circ-30^\circ], [30^\circ-45^\circ], [45^\circ-60^\circ]\) and \([60^\circ-90^\circ]\). Five pull-out curves were then calculated for orientation angles \(0^\circ, 15^\circ, 30^\circ, 45^\circ\) and \(60^\circ\), and assigned for each group respectively. The pull-out curves were calculated using the theoretical average value of the embedded length, \(l/4=3.25\text{mm}\) (Cunha et al., 2012; Li et al., 1991), and the experimental data in (Lee et al., 2010) with parameters presented in Table 3.1.
6.3 Modelling of the in-situ wedge splitting test

6.3.1 Finite element model

Figure 6.3 sketches the specimen used in the in-situ μXCT wedge splitting test and the loading condition. The splitting horizontal force \( F_1 \) acting on the roller bearing can be calculated from simple force balance equations taking the wedge angle and frictional forces into consideration using (Rossi et al., 1991):

\[
F_1 = \frac{F}{2 \tan \varphi} \cdot \frac{1 - \mu \tan \varphi}{1 + \mu \cot \varphi} \approx \frac{F}{2 \tan \varphi} \cdot \frac{1}{1 + \mu \cot \varphi}
\]  

(6.7)

where \( \varphi \) is the wedge angle and \( \mu \) is the coefficient of friction. The effect of frictional forces of the bearing rollers can be neglected assuming its contribution is quite small (Rossi et al., 1991; Walter et al., 2005). Thus equation (6.7) can be reduced to:

\[
F_1 = \frac{F}{2 \tan \varphi}
\]  

(6.7)

where \( \varphi = 17^\circ \) in this test, leading to \( F_1 = 1.63F \). The lower roller supports were modelled by restricting the vertical displacement (along z-axis) of the corresponding nodes as shown in Figure 6.3b. The loading was applied on the corner nodes of the groove. The finite element analysis was conducted using ABAQUS/implicit solver version 6.12.

![Free body diagram of forces.](image1)

![Applied loads and boundary conditions.](image2)

Figure 6.3 The developed model for the wedge splitting test showing the applied load and the boundary conditions.
6.3.2 Results and discussion

The mortar was modelled by tetrahedron elements C3D4. A mesh convergence study with three mesh sizes: 1mm, 0.5mm and 0.2mm in the specimen centre was carried out first. The number of elements are 33229, 121091 and 1184542 and the number of nodes are 6282, 22380 and 204723 respectively for the three meshes as shown in Figure 6.4.

Figure 6.4 Meshes for the mortar matrix with three different sizes at the centre.

Figure 6.5 compares the load versus crack width curves from the three meshes. It can be seen that the predicted ultimate load is virtually identical. The post peak response of the coarse mesh is slightly higher than those of the medium and fine meshes.

Figure 6.5 Load-crack width curves for the different mesh sizes.
The effect of mesh size on the crack path is illustrated in Figure 6.6. The red elements represent the elements that are completely failed with SDEG close to 1. It can be seen that the crack paths from all three meshes are inclined towards the right support, similar to the tested specimens, as shown in Figure 4.4. The un-symmetric crack path is attributed to the random distributions of discontinuous short fibres. To clarify this point, the models were re-simulated without fibres and the crack paths are illustrated in Figure 6.7 for the coarse and medium meshes. It can be seen that the crack paths are nearly vertical. This reflects the significant effects of distribution of the fibre orientation on the predicted crack paths, and thus the importance of using the real fibre distribution in mesoscale numerical models. It is worth noting that macroscopic models, that assume UHPFRC as one homogeneous material can only predict symmetric crack paths (Mahmud et al., 2013).
Figure 6.6 The simulated crack paths from different meshes.
Figure 6.7 The simulated crack paths in unreinforced mortar.

Figure 6.8 compares the numerically predicted load versus the crack opening displacement curve with the experimental data in Figure 4.34 measured from the µXCT images. The numerical curve for the unreinforced specimen is also plotted. It can be seen that the load from the model without fibres decreased sharply after the peak, whereas the UHPFRC model predicted much more ductile behaviour. The peak load for the model with fibres is slightly higher than that without fibres, and close to the experimental load at the end of the linear stage. The post peak responses of numerical and experimental curves are different, probably due to the indirect modelling of fibre-mortar interfaces by 1D embedded elements with equivalent elasto-plastic constitutive relation. The results can be improved by more realistic representation of the fibre-mortar interfaces.
6.6 Summary

In this chapter, a nonlinear FE model has been developed to simulate the in-situ μXCT wedge splitting test presented in Chapter 4. The fracture behaviour of the mortar matrix was simulated using the concrete damage plasticity model in ABAQUS. The fibres with actual distribution in the in-situ specimen were modelled. The pull-out behaviour was modelled indirectly by specifying equivalent tensile constitutive laws for the fibres, which were embedded within the mortar mesh with perfect bond. The predicted crack paths have a good agreement with the experimental data, however, the models have limited success in predicting the loading responses. The results showed the significant effects of fibre orientations on the crack propagation direction.
Chapter 7: Conclusions and Future Works

7.1 In-situ µXCT experiments

The µXCT has been used to conduct in-situ tests for notched UHPFRC specimens under progressive wedge splitting loading for a better understanding of fracture behaviour and toughening mechanisms. The complicated fracture features were visualised and characterised in details with 16.9µm voxel resolution, using 2D µXCT images and 3D volumes.

The results have demonstrated the significant effects of fibres in stabilizing the cracks in the mortar and suppressing them from propagation, which leads to nonlinear strain hardening in the loading curve after the first cracking up to the ultimate strength. The results have also showed the significant effects of the fibre orientation on the crack paths. The cracks tend to propagate parallel to the fibres in the fibre-mortar interfaces, which has made the crack path deviate away from its originally vertical orientation towards the overall fibre direction crossing the cracks.

Bending of inclined fibres has also been observed clearly in the µXCT images at very early stage of cracking. While fibre pull-out phenomenon has been seen at relatively wide cracks. Not all the fibres are pulled out from their shorter embedded length, reflecting the dependency of the pull-out behaviour on the structure of the surrounding matrix. At wider cracks, spalling of the mortar has also been observed at the crack surfaces.

The toughening mechanisms of short random fibres in the UHPFRC are very complex. This study shows that the µXCT technique can play a critical role in providing a detailed and informative interpretation of these mechanisms.

Another µXCT scan has been conducted for a 20mm UHPFRC cube with a resolution of 24.8µm. The numbers, shapes, volume fractions and distributions of both steel fibres and pores are all visualised and determined by analysing the µXCT images from both scans. The fibre volume fractions are 3.75% and 2.57% for the specimen used in the first in-situ test and the 20mm cube specimen respectively, and the pore volume fractions are 2.99% with diameters ranging from 25-1400µm and 2.55% with diameters between 40-1800 µm, respectively. Although the resolution in the 20mm cube scan (24.8µm) is lower than
the in-situ test scan (16.9µm), smaller pores are detected in the former due to the enhanced contrast. The different fibre contents in both scanned specimens, which are segmented based on the diameter of the steel fibres (0.2mm), reflect the non-uniform distributions of fibres in the original beam, from which the µXCT specimens were cut.

7.2 Numerical modelling
In this study, three different finite element approaches to model the mechanical behaviour of UHPFRC with discrete fibre representation have been proposed. Firstly, 2D mesoscale models were developed to simulate the tensile fracture behaviour of the UHPFRC. Discrete cracks in the mortar were modelled using zero-thickness CIEs that were pre-inserted in the mortar mesh. The fibres with random distribution were generated using an in-house Matlab code as two-noded elements. Each fibre was split into segments at the intersections with the CIEs. Nonlinear spring-like elements were inserted between the fibre segments to bridge the CIEs and simulate the pull-out behaviour of fibres. The pull-out relation of each fibre was calculated as a function of its orientation angle and embedment length, using an analytical pull-out model and employed to define the constitutive laws of the connector elements. Discrete crack representation, which gives definite crack paths and directions, make direct use of the fibre orientations and embedded lengths, leading to accurate calculations of the pull-out relations. This modelling approach thus offers a direct link between fibre local pull-out behaviour and the composite response at the macroscale and can be used to conduct parametric studies for the optimisation of the UHPFRC.

Secondly, a two-scale analytical-numerical homogenisation method has been developed based on the µXCT images obtained for the 20mm cube. The micro-indentation technique was used to measure the local elastic properties of the constituents of the mortar matrix: silica sand and cement paste. Based on the distribution of pore sizes in the 20mm UHPFRC cube, a two-scale homogenisation approach to calculate the effective elastic properties of the UHPFRC has been developed. The analytical Mori-Tanaka scheme was used in the first scale to homogenise the sand particles, cement paste and the large number of small pores ($d_e < 600\mu$m). In the second scale, 3D mesoscale FE models of RVEs were built directly from the µXCT for numerical homogenisation, with steel
fibres and the small number of large pores ($d_c > 600\mu m$) embedded in the homogenised mortar from the first scale. The coupling of analytical and numerical homogenisation the two scales results in tremendous computational savings over other approaches using numerical homogenisation at both scales. The developed approach thus offers an accurate and efficient tool to conduct parametric studies for optimisation of the material's microstructure for desired mechanical properties.

Thirdly, nonlinear FE models have been developed to simulate the in-situ µXCT wedge splitting test. The concrete damage plasticity model was adopted to simulate the fracture behaviour of the mortar. The fibres were simulated as 1D truss elements with actual positions and orientations, and bonded perfectly with the mortar mesh. The fibre-mortar interfacial behaviour was considered indirectly by equivalent stress-strain curves of fibres converted from the pull-out relations. The results revealed the importance of using the actual fibre orientations and positions to obtain accurate crack path.

7.3 Future research work
The following works are suggested for future study:

(1) developing more powerful image processing software, that can be used to process large datasets automatically without excessive manual interactions and to generate more accurate finite element meshes from the µXCT images;

(2) conducting more µXCT in-situ tests on UHPFRC under different loading conditions such as direct tensile test and three-point bending test. As the mechanical behaviour of the UHPFRC is highly dependent on the fibre-mortar interface, interfacial debonding can be studied using in-situ µXCT pull-out tests of single or multiple fibres;

(3) improving the discrete crack-based model (proposed in Chapter 3) by distributing the connector elements along the fibre axis rather than placing them at specific points. This can be achieved by using conforming meshes for the mortar and fibres, so that the nodes in the mortar mesh coincide with fibre nodes. This will require the development of subroutines in ABAQUS to change the node connectivity during fibre pull-out process
and update the constitutive laws of the connector elements according to the cracks formed in the mortar;

(4) extending the multiscale models (proposed in Chapter 5) to predict the strength and the post peak fracture behaviour of the UHPFRC by considering the fibre pull-out behaviour. This can be achieved by inserting cohesive elements between fibres and the surrounding mortar. The fracture behaviour of the mortar can be modelled either based on discrete crack approach, or smeared crack approach;

(5) improving the finite element models of in-situ wedge splitting tests by more realistic modelling of the fibre-mortar interface. For 1D fibre elements, the bond can be modelled using connector elements distributed along the fibre elements as explained in (3) above. However, more accurate framework can be developed by simulating fibres as 3D cylinders, and modelling the fibre-mortar interface using discrete crack model as explained in (4).
References


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