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Micro X-ray computed tomography image-based two-scale homogenisation of ultra high performance fibre reinforced concrete

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HIGHLIGHTS

- Micro X-ray computed tomography (μXCT) images obtained for UHPFRC with 24.8 μm resolution.
- A two-scale homogenisation method developed for UHPFRC based on CT images and pore sizes.
- The homogenised elastic moduli compared satisfactorily with experimental data.
- The method's capability of optimising fibre orientation and volume fraction demonstrated.

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ABSTRACT

A two-scale analytical-numerical homogenisation approach is developed to predict effective elastic properties of ultra high performance fibre reinforced concrete considering distribution of pore sizes acquired from 3D micro X-ray computed tomography (μXCT) images of 24.8 μm resolution. In the first scale, the mortar, consisting of sand, cement paste and a large number of small pores (10–600 μm), is homogenised using analytical Mori-Tanaka method with constituents' moduli from micro-indentation. In the second, μXCT images of a 20 mm cube are converted to mesoscale representative volume elements for finite element homogenisation, with fibres and a small number of large pores (⩾600 μm) in the homogenised mortar. The resultant elastic moduli are compared favourably with experimental data. This approach accounts for a large number of pores with a wide size range yet without excessive computational cost. Effects of fibre volume fraction and orientation are investigated, demonstrating the approach's potential to optimise the material's micro-structure for desired properties.

1. Introduction

Ultra high performance fibre reinforced concrete (UHPFRC) or reactive powder concrete has many advantages over conventional concrete, fibre reinforced concrete (FRC) and high performance concrete, including considerably higher ductility, durability and strength (typically over 150 MPa in compression and 9 MPa in tension) [1,2]. These properties are achieved using a high cement content, low water/cement ratio (<0.2), fine silica sand (size <0.5 mm), microsilica or silica fume, superplasticizer and other additives, resulting in a very dense cementitious matrix. Short (3–13 mm), high strength (typically 2000 MPa) steel fibres of 1–10% volume fraction are also added, leading to very high fracture energy (up to 40,000 J/m^2), little size effect in bending [3] and excellent impact and blast resistance [4–6].

Although the material has been used in many special structures and components, its wide applicability so far is limited, mainly due to relatively high material costs and lack of widely-accepted design codes [7]. This situation can be improved with a better understanding of the relationships between the material's internal structure and mechanical properties at micro-, meso- and macro-scales, so that the mix design can be optimised for desired performances yet with minimal costs.

Extensive experiments have been carried out to obtain the mechanical properties of UHPFRC [2–6,8,9] and to establish empirical relationships between the overall mechanical properties and the usage of constituents or phases [10,11]. Experiments are often

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extensive, difficult and costly to carry out, especially if the effects of the phase distributions, volume fractions and local micro-structures are investigated.

Several homogenisation techniques, in which a heterogeneous material is replaced by an equivalent homogeneous continuum, have been proposed to evaluate the effective elastic properties of composite materials. A common method is analytical estimating of upper and lower bounds based on the volume fractions and elastic moduli of both matrix and reinforcement, for example, the Voigt's and Ruess's bounds [12] and Hashin and Shtrikman bounds [13]. The Eshelby's equivalent approach [14], based on single ellipsoidal inclusion in an infinite matrix, is widely used as a basis for more sophisticated analytical homogenisation approaches, such as the Mori-Tanaka (MT) scheme [15,16], the self-consistent approach [17] and the generalized self-consistent scheme [18].

In recent years, having recognised that the mechanical properties of cementitious composites at macro-scale are highly dependent upon the nano/micro-structures and respective properties of individual constituents, researchers have made considerable efforts in developing multiscale models using the above analytical homogenisation techniques (mainly Mori-Tanaka scheme), in which the results obtained at small scale are up-scaled to predict the behaviour at larger scales. For example, multiscale models for estimation of elastic properties have been built for cement paste [19,20], mortar and concrete [21–23] and UHPFRC [24]. Although simple and efficient, these analytical models (whether multiscale or not) cannot consider the complicated, realistic shapes, size gradations, and random distribution of the inclusions due to simplifications necessary for analytical derivations.

An alternative to analytical approaches is numerical homogenisation, mostly using the finite element method (FEM) capable of modelling complicated heterogeneous material structures at different length scales. This approach allows homogenisation of macro-scale properties from numerical solutions of a representative volume element (RVE) [25]. Although widely used to study composite materials, its application to cementitious materials is limited. Recently a few two-step homogenisation approaches have been developed for FRC [26,27], in which the inclusions (fibres and aggregates) and surrounding interfacial zone are homogenised first using Gaboczi's analytical method [28], and the homogenised inclusions are then integrated with the mortar matrix to predict overall elastic properties of FRC using numerical homogenisation. In these studies, the material's micro-structures used in the second step are generated using statistical algorithms with inclusions of simplified shapes and distributions, and little attention is paid to the effects of pores which exist intrinsically in cementitious composites. One important reason is the lack of real 3D internal micro-structures, and another is the high computational cost caused by explicit modelling of constituents in the micro-structures.

Recently, micro X-ray computed tomography (µXCT), a 3D imaging technique routinely used in hospitals, has become popular in characterising the internal nano-, micro- and meso-scale structures of many materials, because of its high resolution, non-destructive nature, and clear visualisation of shapes, sizes and distribution of multi-phases including pores and cracks. For example, µXCT has been used to characterise metals and alloys [29,30], porous materials [31], snow [32], nuclear graphite [33], composites [34], asphalt mixtures [35], and concrete [36–38]. It has also been used to examine fibre reinforced composites such as glass fibre reinforced polymer [39] and carbon/carbon composites [40]. A few studies have used µXCT to characterise the structure and behaviour of FRC, e.g., on fibre orientations [41,42], fibre spacing [43], and measurement of fracture energy [44].

This study aims at developing an accurate and efficient two-scale homogenisation approach for the prediction of elastic properties for fibre reinforced concrete such as UHPFRC. The 3D micro-structure of a 20 mm UHPFRC cube with a voxel resolution of 24.8 µm is obtained by µXCT scanning. Statistical analysis of the pore sizes in the µXCT images is then carried out based on which a two-scale homogenisation approach is developed. At the first scale, the mortar is considered as a three-phase material composed of cement paste (containing the hydrated CSH, un-hydrated cement clinkers, GGBS and silica fume), silica sand and a large number of small pores smaller than 600 µm. The elastic properties of the cement paste and silica sand are obtained by micro-indentation tests. At the second scale, UHPFRC is modelled as a three-phase material with the homogenised mortar, steel fibres and a small number of pores larger than 600 µm. A different homogenisation approach is used in each scale: the analytical Mori-Tanaka average stress theory is used in the mortar step to avoid modelling the large number of small pores as in numerical homogenisation, while numerical homogenisation using 3D FE models transformed directly from µXCT images is used in the second scale. The developed method thus combines the efficient analytical approach and the realistic numerical approach. The steel fibres are modelled by both 3D solid elements and 1D truss elements. The effects of RVE size, volume fraction and orientation of steel fibres on the elastic moduli are also investigated.

2. Experimental studies

2.1. Materials and basic properties

The mix design of UHPFRC investigated in this study, summarised in Table 1, was developed at the University of Liverpool [2,8,9], where the detailed fabrication process could be found. The straight steel fibres are of 2000 MPa in strength, 13 mm in length and 0.2 mm in diameter with a volume fraction $f_f = 2\%$.

A 20 mm cube was cut from one of the UHPFRC beams cast for a size-effect investigation [3] and used in this study. The basic properties of the material at 28 days from standard tests are [2]: compression strength 150.56 MPa, tensile strength 9.07 MPa, and Young's modulus 45.55 GPa. They are 121.32 MPa, 5.36 MPa and 42.08 GPa, respectively for the UHPC without steel fibres.

2.2. µXCT scanning, segmentation and image analyses

The 20 mm cube was scanned at the Henry Moseley X-ray Imaging Facility, the University of Manchester, UK, using a Nikon XTEK XTH 225 kV machine with 130 kV and 110 µA intensity. The stage was rotated by 360°, resulting in 2985 2D radiographs with an angular displacement 0.1206° and a pixel resolution 24.80 µm. The scan took about 17 min. The 2D radiographs were then reconstructed into 3D absorption contrast image of the sample using the CT Pro and VG Studio software. Artificial defects such as beam hardening and ring effects were removed by post-processing. Fig. 1a is a 2D µXCT image slice showing the mortar in grey, the fibres in white and the pores in black. A reconstructed

Table 1
Details of the UHPFRC Mix [2].

Mix content	kg/m^3
Cement	657
Ground Granulated Blast Furnace Slag (GGBS)	418
Microsilica (silica fume)	119
Silica sand (average diameter 0.27mm)	1051
Superplasticizer	40
Water	185
Steel fibre, $f_f = 2\%$	157
Total	2627