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Application of X-ray computed tomography on fracture behaviour study of cement paste at micro-scale

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Micro Abstract
3D microstructure with a cubic dimension of 100 μm^3 was generated by X-ray computed tomography. Its mechanical properties were predicted by the microstructure informed lattice model. Considering the heterogeneous nature of this material, 30 specimens were investigated. Correlation analysis was conducted between the simulated mechanical properties and porosity.

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Introduction

Cement paste is a porous and heterogeneous material. As the basic material in concrete, it has generated considerable research interest. It is generally accepted that its fracture properties, i.e. tensile strength and elastic modulus largely depend on its material structure at micro-scale which locally shows a notable variation [2]. For a number of reasons that include problems with producing and measuring miniaturized mechanical samples, direct measurement of micromechanical properties can be hardly achieved experimentally so far. Despite this, application of microstructure informed numerical model offers an unprecedented opportunity to achieve this. Such models mainly require the detailed microstructure and micromechanical properties of individual phases in the microstructures. In this paper, a method combined discrete lattice fracture mode [1] and X-ray computed tomography (XCT) is described to predict the micromechanical properties of cement paste. Considering the heterogeneous nature of this material, 30 microstructures with a cubic dimension of 100 μm^3 are investigated. The strength distribution and its relationship with elasticity are studied by statistical analysis. A correlation is conducted between the predicted strength and porosity.

1 Materials and experiments

In the experimental program, small cement paste prism with cubic cross-section of 500 μm $\times$ 500 μm was produced and scanned by a Phoenix Nanotom microcomputed tomography system. Cement pastes were prepared with standard grade CEMI 42.5N Portland cement and deionized water. The w/c ratios of used paste were 0.3, 0.4 and 0.5. The fresh cement mixture was sealed in a cylindrical module. After 28 days hydration, the specimens were first cut into 2 mm slices and then grounded down to 500 μm. The small prism was then prepared by running a micro dicing saw (MicroAce Series 3 Dicing Saw) over the thin section. A special holder was used to clamp the small prism during scanning. 2800 projections were acquired on a digital GE DXR detector (3072 $\times$ 2400 pixels) under 12 kev/60 μA of X-ray source to reach a spatial resolution of 0.5 $\times$ 0.5 $\times$ 0.5 μm^3. The software Phoenix Datos|x was used for the reconstruction work. For saving the computational efforts on fracture behaviour modelling, the resolution was reduced to 2 μm^3/voxel. Four phases (pore, anhydrous cement, inner hydration products and out hydration products) were isolated using global threshold method. More details about the image processing

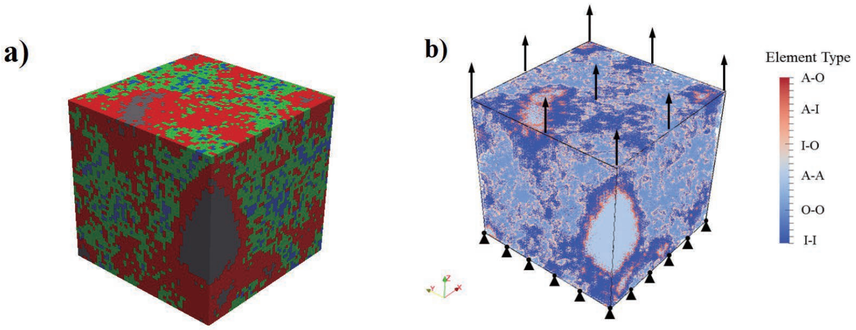

Figure 1. (a) 3D segmented microstructure of cement paste (grey-anhydrous cement; red-inner product; green-outer product; blue-pore); (b) uniaxial tensile test on lattice mesh.

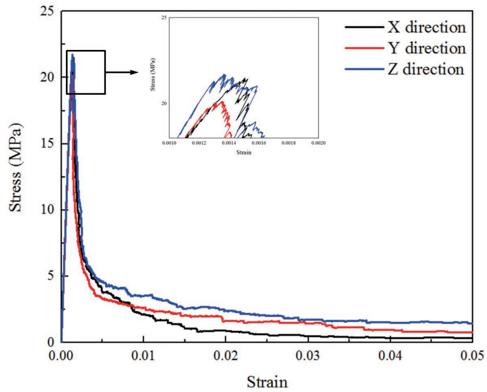

Figure 2. Comparison of simulated stress strain curves of one specimen under uniaxial tension from three directions.

can be found in [3]. For each w/c ratio, 10 microstructures in a shape of cube (100 μm^3) as shown in Figure 1a were randomly extracted from the segmented images. Volume fraction of pore phase was used to present the porosity of each investigated microstructure.

2 Modelling

For the deformation and fracture analysis, a lattice type model, as described in [1], was used. In the lattice model, the material was discretized as a set of beam elements. Then, a set of linear elastic analyses was performed by calculating the nodal responses of the lattice network for a uniaxial tensile test boundary condition as shown in Figure 1b. In each analysis step, only a single beam element is removed from the mesh, thereby introducing a small crack. The analysis is then repeated with the updated geometry and stiffness of the whole lattice network until a pre-determined failure criterion is reached. A single virtual specimen was loaded along three directions, and as the investigated microstructure is not ideal isotropic homogeneous, the simulated mechanical properties are expected to be different. As an example,the stress-strain responses and crack patterns of one virtual specimen are shown in Figure 2 and Figure 3 respectively. The modulus and strength can be then calculated from the stress-strain curve.

3 Results and Discussion

A two parameter Weibull statistic was used to analyse the fracture data for specimens in each w/c group. The probability of failure can be written as:

$$\ln\ln\left(\frac{1}{1-P_f}\right) = \ln\sigma_f - \ln\sigma_c \tag{1}$$

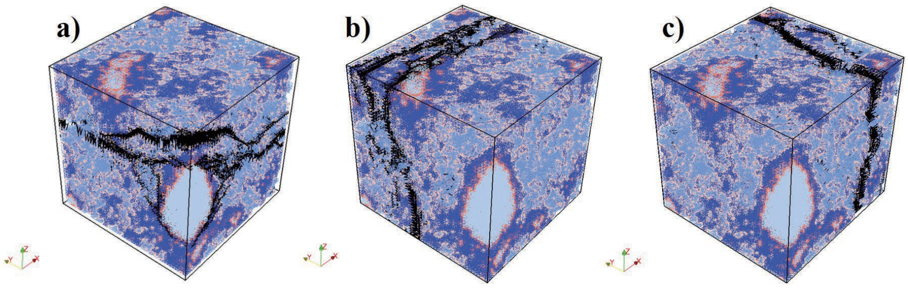

Figure 3. Crack pattern of cement paste under uniaxial tension in three directions: (a) Z (b) Y and (c) X. (black-cracked element; Deformations have been scaled for clarity).

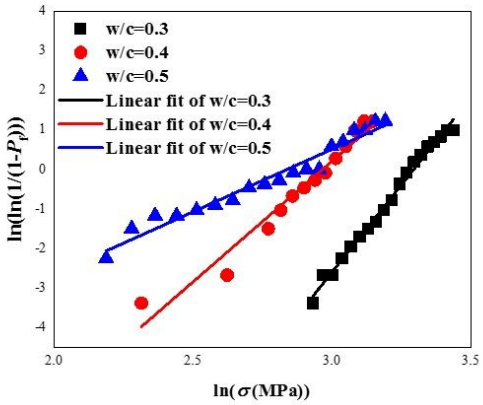

Figure 4. Weibull plot for simulated tensile strength of cement paste with different w/c ratios.

where P_f is the cumulative probability of failure and m is the Weibull modulus. Also, σ_f is the fracture strength and σ_c is the Weibull scale parameter. The tensile strengths are plotted in a Weibull coordinate system (Figure 4). The least squares method was adopted to fit the Weibull modulus and scaling parameter. The fitted results are given in Table 1. A coefficient of determination (R^2) higher than 0.9 is observed for all w/c ratios. Both Weibull modulus and scaling parameter decreases with the increase of w/c ratio, which indicates that pore structures are clustered more inconsistently in paste specimens with higher w/c ratios. The ratio between elastic modulus and strength is then plotted against strength in Figure 5. Although a relatively wide range from 800 to 1800 is observed, it is evident that this ratio decreases with the increased strength value. Furthermore, two linear boundaries can be defined using the least squares method and it is interesting that the two bounds are quite paralleled to each other, which deserves further study. The mean value of strengths in three directions of one sample is used for the empirical strength-porosity relationship study. As shown in Figure 6, four types of empirical model are fitted. The exponential curve yields the highest determination coefficient value. The predicted results in forms of exponential and power are quite close to each other and predict the strength of non-porosity cement paste to be around 36 MPa and 37 MPa. Furthermore, the Logarithmic model determines a critical porosity value as 60.57 % in which the material yields zero strength.

W/c ratio	Weibull modulus	Weibull scale	Determination coefficient
0.3	8.85	26.96	0.99
0.4	6.11	19.41	0.98
0.5	3.17	17.10	0.96

Table 1. Weibull parameters for the simulated tensile strength

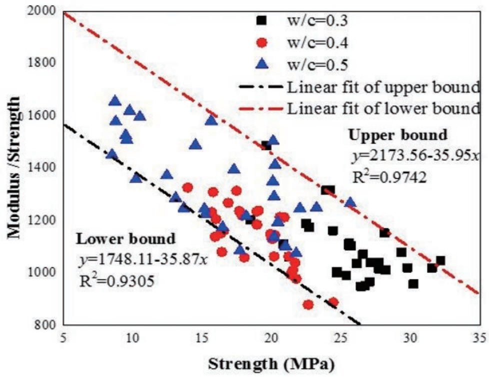

Figure 5. Relationship between predicted modulus/strength ratio and strength.

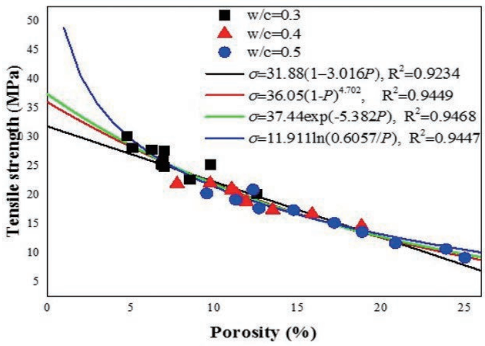

Figure 6. Relationship between predicted tensile strength and porosity.

Conclusions

Based on the XCT generated material structure of cement paste, the micromechanical properties of this material were predicted by the discrete lattice fracture model. Although the current study is limited by the resolution and computational resources, the following conclusions can be drawn:

With w/c ratio decreasing, the Weibull modulus and scaling parameter increases, which indicates specimens with lower w/c ratio generally yield a stronger and less variable fracture performance.

The ratio between elastic modulus and strength decreases with the increased strength.

Porosity appears to be the main factor determining the strength of cement paste. Over the examined porosity range from 5 % to 25 %, the existing sample empirical equation in form of exponential can be regarded as a good representation on the predicted strength of cement paste at micro-scale.

Acknowledgements

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