Multiscale Material Design and Crack Path Prediction of a Cementitious Cover Layer with High Toughness

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ABSTRACT. *A new kind of cementitious composite with high toughness, which is used as the cover layer of bridge and highway, is examined by means of the multiscale material design theory. The primary mechanical properties and the crack path of the designed cementitious composite are predicted by a revised lattice model based on the meso-structure of the cementitious composite scanned by a micro-CT (micro-focus computational tomography). Further, the reliability of the modeling results is verified by laboratory experimental test results. The primary mechanical properties of the designed cementitious cover layer are obtained from static bending tests. The results show that multiscale components of the cementitious composites can be effectively selected and optimized by the multiscale material design theory. Finally, the optimized mix proportion and the appropriate latex additions are determined for the cementitious cover layer with high toughness.*

1. INTRODUCTION

Because of the brittleness of cementitious materials, the cover layers of both highway and bridge are usually made of asphalt-based concrete which presents high toughness. With the shortage of petroleum around the world, the usage of asphalt for cover layer composite is negative as far as the energy consumption and environment protection are concerned. Therefore, cementitious composites, characterized by high toughness and low dosage of Portland cement, can be produced for this purpose, such as the polymer concrete [1], latex-modified concrete [2], crumb rubber concrete [3], fly ash concrete [4], fiber reinforced concrete [5], etc. Although the types of toughening admixtures are various, their toughening mechanism on cementitious composites is the same, that is, optimization of the material parameters of multiscale components. However, the theoretical material design of cementitious composites toughened by liquid polymer or liquid latex is more difficult than that of composites toughened by fiber or crumb rubber.

Therefore, the multiscale design method is employed to reliably prepare the cementitious cover layer toughened by the liquid latex. The primary mechanical properties and failure behaviour of the designed cementitious cover layer are predicted by a revised lattice model based on the real meso-structure image of the designed composite. In order to determine an optimized mix proportion for the designed cementitious cover layer, the prediction results of the numerical simulation are compared with the laboratory mechanical test results.

2. MULTISCALE MATERIAL DESIGN

2.1 Theoretical Background

The designed cementitious composites are composed of mortar matrix and coarse aggregate. The mortar matrix also includes two elements, i.e. hardened cement paste, fine aggregate. Therefore, the relations between the volume fractions of each component are expressed in Eq. (1) and Eq. (2).

Macro-scale $v_m + v_{ca} = 1$ (1)

Meso-scale $v_c + v_{fa} = 1$ (2)

where v_m, v_{ca}, v_{fa}, v_c is the volume fractions of mortar matrix, coarse aggregate, fine aggregate and hardened cement paste, respectively. For a composite material, the stress-strain relationships of the cementitious composite and the components are as follows [6]:

Composite element $\{s\} = [q]\{e\}$ (3)

Mortar matrix element $\{s_m\} = [q_m]\{e_m\}$ (4)

Coarse aggregate element $\{s_{ca}\} = [q_{ca}]\{e_{ca}\}$ (5)

Fine aggregate element $\{s_{fa}\} = [q_{fa}]\{e_{fa}\}$ (6)

Hardened cement paste element $\{s_c\} = [q_c]\{e_c\}$ (7)

Based on the assumption of plane stress, the equivalent stiffness is expressed as

$$[q] = E_u \begin{bmatrix} 1 & u & 0 \\ u & 1 & 0 \\ 0 & 0 & \frac{1-u}{2} \end{bmatrix} \tag{8}$$

$$E_u = \frac{E}{1-u^2} \tag{9}$$

where $\{s\}, \{e\}$ and $[q]$ are the stress, the strain and the stiffness matrix, respectively. Further, E is the elastic modulus, u is the Poisson's ratio.

The mean volume stress and strain of the multiscale elements are defined as [6]:

Macro-scale element $\{s\} = v_m\{s_m\} + v_{ca}\{s_{ca}\}$ (10)

$\{e\} = v_m\{e_m\} + v_{ca}\{e_{ca}\}$ (11)

Meso-scale element $\{s_m\} = v_c\{s_c\} + v_{fa}\{s_{fa}\}$ (12)

$\{e_m\} = v_c\{e_c\} + v_{fa}\{e_{fa}\}$ (13)

Therefore, if the mechanical properties of coarse and fine aggregates are available in advance, the primary material parameters (such as elastic modulus, Poisson’s ratio, etc.) of other meso-scale components could be predicted according to the macroscopic stress-strain relationship of the cementitious composite.

2.2 Material Design of Cementitious Cover Layer

The proposed cementitious cover layer should endure the maximum tensile stress equal to 10 MPa. The elastic modulus of the proposed composite should be 30 GPa. The Poisson’s ratio of the macro-scale composite and of the mortar matrix is 0.2. The crushed basalt with density of 2590 kg/m^3 and quartz sand with density of 2630 kg/m^3 are used as the coarse aggregate and the fine aggregate, respectively. The volume fraction is proposed to be 38% for coarse aggregate in macro-scale composite, and 42% for fine aggregate in mortar matrix. The tensile strength of basalt and that of quartz stone are 30 MPa and 10 MPa, respectively. The elastic modulus is 160 GPa for coarse aggregate and 78 GPa for fine aggregate, and the Poisson’s ratio is 0.1. The composite is designed by following three steps.

2.2.1 Step I – Calculations on the primary material parameters of mortar matrix

- *The equivalent stiffness of cementitious cover layer and coarse aggregate*

When $E = 30GPa, u = 0.2, E_{ca} = 160GPa, u_{ca} = 0.1$, then we get

$$[q] = \begin{bmatrix} 31.3 & -6.3 & 0 \\ -6.3 & 31.3 & 0 \\ 0 & 0 & 12.5 \end{bmatrix} (GPa) \tag{14}$$

$$[q_{ca}] = \begin{bmatrix} 161.6 & -16.2 & 0 \\ -16.2 & 161.6 & 0 \\ 0 & 0 & 72.7 \end{bmatrix} (GPa) \tag{15}$$

- *The maximum strain of cementitious cover layer and coarse aggregate*

When $s_1 = 10MPa, s_{1,ca} = 30MPa$, we get

$$\{e\} = [q]^{-1}\{s\} = \begin{bmatrix} \frac{1}{30} & -\frac{1}{150} & 0 \\ -\frac{1}{150} & \frac{1}{30} & 0 \\ 0 & 0 & 0.08 \end{bmatrix} \times 10^{-9} \cdot \begin{bmatrix} 10 \times 10^{6} \\ 0 \\ 0 \end{bmatrix} = \begin{Bmatrix} 333.3 \times 10^{-6} \\ -66.7 \times 10^{-6} \\ 0 \end{Bmatrix} \tag{16}$$

$$\{e_{ca}\} = [q_{ca}]^{-1}\{s_{ca}\} = \begin{bmatrix} \frac{1}{160} & -\frac{1}{1600} & 0 \\ -\frac{1}{1600} & \frac{1}{160} & 0 \\ 0 & 0 & 0.01 \end{bmatrix} \times 10^{-9} \cdot \begin{bmatrix} 30 \times 10^{6} \\ 0 \\ 0 \end{bmatrix} = \begin{Bmatrix} 187.5 \times 10^{-6} \\ -18.8 \times 10^{-6} \\ 0 \end{Bmatrix} \tag{17}$$

- *The predicted material parameters of mortar matrix*

Based on Eq. (3) to (5), Eq. (1) and Eq. (10), the relationship of macro-scale strain and coarse aggregate strain is as follows:

$$\{e\} = v_{ca}\{e_{ca}\} - v_{ca}([q]-[q_m])^{-1} \cdot ([q]-[q_{ca}])\{e_{ca}\} \tag{18}$$

When $v_{ca} = 38\%$ and $u_m = 0.2$, the elastic modulus of mortar matrix is computed to be about 17 GPa from Equations (14) to (18). Then, the equivalent stiffness of the mortar matrix is

$$[q_m] = \begin{bmatrix} 17.7 & -3.5 & 0 \\ -3.5 & 17.7 & 0 \\ 0 & 0 & 7.1 \end{bmatrix} (GPa) \tag{19}$$

■ *The predicted tensile strength of mortar matrix*

When $v_{ca} = 38\%$, $v_m = 1 - v_{ca} = 62\%$, the strain of mortar matrix is computed from Eq. (11):

$$\{e_m\} = \begin{Bmatrix} 422.7 \times 10^{-6} \\ -96.1 \times 10^{-6} \\ 0 \end{Bmatrix}. \tag{20}$$

According to Eq. (4), the maximum tensile stress of mortar matrix is

$$\{s_m\} = \begin{Bmatrix} s_x \\ s_y \\ t_{xy} \end{Bmatrix} = [q_m]\{e_m\} = \begin{bmatrix} 17.7 & -3.5 & 0 \\ -3.5 & 17.7 & 0 \\ 0 & 0 & 7.1 \end{bmatrix} \times 10^9 \cdot \begin{Bmatrix} 422.7 \\ -96.1 \\ 0 \end{Bmatrix} \times 10^{-6} = \begin{Bmatrix} 7.8 \\ -3.2 \\ 0 \end{Bmatrix} (MPa) \tag{21}$$

Therefore, the mortar matrix should be designed with the following parameters: $E_m = 17GPa$, $v_m = 0.2$, $s_{1,m} = 7.8MPa$.

2.2.2 Step II – Calculations on the primary material parameters of hardened cement paste

■ *The equivalent stiffness of fine aggregate*

When $E_{fa} = 78GPa, v_{fa} = 0.1$, the equivalent stiffness of fine aggregate can be computed according to Eq. (8) and Eq. (9).

$$[q_{fa}] = \begin{bmatrix} 78.8 & -7.9 & 0 \\ -7.9 & 78.8 & 0 \\ 0 & 0 & 35.5 \end{bmatrix} (GPa) \tag{22}$$

■ *The maximum strain of fine aggregate*

When $s_{1,fa} = 10MPa$, the strain of fine aggregate can be computed from Eq. (6).

$$\{e_{fa}\} = [q_{fa}]^{-1}\{s_{1,fa}\} = \begin{bmatrix} \frac{1}{78} & -\frac{0.1}{78} & 0 \\ -\frac{0.1}{78} & \frac{1}{78} & 0 \\ 0 & 0 & 0.03 \end{bmatrix} \times 10^{-9} \cdot \begin{bmatrix} 10 \times 10^6 \\ 0 \\ 0 \end{bmatrix} = \begin{Bmatrix} 128.2 \times 10^{-6} \\ -12.8 \times 10^{-6} \\ 0 \end{Bmatrix} \tag{23}$$

■ *The predicted material parameters of hardened cement paste*

When $v_{fa} = 42\%, v_c = 1 - v_{fa} = 58\%$, the strain of hardened cement paste is computed from Eq. (13), (20) and (23):

$$\{e_c\} = \begin{Bmatrix} 636.0 \times 10^{-6} \\ -156.4 \times 10^{-6} \\ 0 \end{Bmatrix}. \tag{24}$$

Equation (12) can be rewritten:

$$v_c[q_c]\{e_c\} = \{s_m\} - v_{fa}[q_{fa}]\{e_{fa}\} \tag{25}$$

Based on Eqs (2), (4), (6), (7) and (12), the elastic modulus of the hardened cement paste is given by:

$$[q_c] = \frac{1}{v_c}[\{s_m\} - v_{fa}\{s_{fa}\}] \cdot \{e_c\}^{-1} \tag{26}$$

Substituting Eq. (20) to (23) into Eq. (26), the elastic modulus and Poisson's ratio of the hardened cement paste are 12 GPa and 0.25, respectively. Then, the equivalent stiffness of hardened cement paste is

$$[q_c] = \begin{bmatrix} 12.6 & -3.2 & 0 \\ -3.2 & 12.6 & 0 \\ 0 & 0 & 4.7 \end{bmatrix} (GPa) \tag{27}$$

■ *The predicted tensile strength of hardened cement paste*

$$\{s_c\} = [q_c]\{e_c\} = \begin{bmatrix} 12.6 & -3.2 & 0 \\ -3.2 & 12.6 & 0 \\ 0 & 0 & 4.7 \end{bmatrix} \times 10^9 \cdot \begin{Bmatrix} 636.0 \\ -156.4 \\ 0 \end{Bmatrix} \times 10^{-6} = \begin{Bmatrix} 8.5 \\ -4.0 \\ 0 \end{Bmatrix} (MPa) \tag{28}$$

Therefore, the hardened cement paste should be designed with the following parameters: $E_c = 12GPa, v_c = 0.25$, $s_{1,c} = 8.5MPa$.

2.2.3 Step III – Mix proportion design for cementitious composites

■ *Mix proportion design for cement paste*

The P•Ⅱ42.5 Portland cement with density of 3150 kg/m^3 is used as the main cementitious material. Class F fly ash (FA) with density of 2380 kg/m^3 is used as part of the cementitious material. The specific surface area is 309 m^2 / kg for Portland cement and 665 m^2 / kg for FA. The A-800S water dispersible latex powder supplied by Nanjing Alsdee Chemical Co., Ltd. is used as the chemical toughening agent of the cement paste. The powdery defoaming agent is used for eliminating the air bubble introduced by the dispersible latex. The mix proportion of raw materials for the designed cement paste is listed as follows. The mass fraction of Portland cement and FA is 70% and 30% of the total cementitious material, respectively. The water-binder ratio (i.e. the ratio between water and total cementitious material in mass) is designed to be 0.38. The mix proportion of latex powder and defoaming agent is 3% and 0.3% mass fraction of the total cementitious material, respectively.

The cement paste is cured in the standard curing room (temperature 20 °C ± 2 °C, relative humidity 95%) for 7 days. After curing age equal to 7 days, the hardened cement paste is put into natural environment with temperature 20 °C ± 2 °C and relative humidity 55% for 21 days. The hardened cement paste with hydration age of 28-days is used for mechanical evaluation. Based on the above mix proportions, the primary mechanical properties of the designed cement paste with hydration age of 28-days are: $E_c = 11.5GPa, s_{1,c} = 8.87MPa$. It is clear that these parameters of the hardened cement paste are consistent with the designed ones mentioned above.

■ *Mix proportion design for mortar*

The particle size of continuous grading sand is 0 mm to 5 mm. The sand-cement ratio (i.e. the ratio between sand and Portland cement in mass) is designed to be 2:1. The water-binder ratio is still fixed to be 0.38. The mix proportion of latex powder and defoaming agent is 3% and 0.3% mass fraction of the total cementitious materials, respectively. The mix proportion of the designed mortar is proposed in Table 1. The curing system of mortar is the same as that of hardened cement paste. The mortar specimens with hydration age of 28 days are used for the mechanical evaluation. The primary properties of the designed mortar are as follows: $E_m = 14.4GPa, s_{1,m} = 7.59MPa$. The values of these primary mechanical parameters of the mortar are close to the designed ones.

Table 1. The proposed mix proportion of mortar

Cement	Fly ash	Sand	Water	latex powder	Defoaming agent
0.7	0.3	2	0.38	0.03	0.003

3. NUMERICAL SIMULATION RELATED TO THE DESIGNED CEMENTITIOUS COMPOSITE

As is shown in Figure 1, a digital image of a typical concrete meso-structure scanned by a micro-focus computational tomography is employed for the numerical simulation on the crack path and mechanical behaviour of the designed cementitious composite. In this image, the particle size of the coarse aggregate ranges from 5mm to 20mm. The volume fraction of coarse aggregate is 38% in the selected concrete. The details of the modelling method are described in Ref. [7]. The different mechanical properties are attributed to each lattice element depending on the zone where the element is located. The regular triangular beam lattice is laid on the digital image with an in-house MATLAB program, whereas the two concrete blocks are discretized with 4-node bilinear plane finite elements. The ABAQUS software is used for the numerical simulation. Along the interface between lattice and homogeneous blocks, the mutual displacements along the 1- and 2-axis are constrained. Two point loads acting downwards along the 2-axis are linearly applied to the two top nodes at the lattice-homogeneous block interfaces (located at a distance along the 1-axis equal to 100 mm).

The beam lattice element is 1mm long, 0.58mm high. The thickness of the lattice element and concrete blocks are assumed equal to the unity. The material parameters of the lattice elements are determined, by applying a series of transformation formulas proposed in Ref. [7], from the corresponding parameters of the designed mortar and the selected coarse aggregate, which are listed in Section 2.2. If the axial stress is larger than the tensile strength, the beam element is assumed to fail. The failed element is not removed from the model. Figure 2 shows the predicted crack paths enlightened in red. Because of the high elastic modulus of the coarse aggregate, the crack paths start from the mortar matrix, and extend along the boundary of coarse aggregate with large size. Furthermore, at the time instant when the lattice element fails, the mean tensile strain of 60 lattice elements at the bottom edge of concrete middle span is equal to 291 με. Thus, the elastic modulus of concrete, which includes the coarse aggregate with particle size from 5mm to 20mm, is predicted to be 34.2 GPa. Since the coarse aggregate with large size would accelerate the extension of the crack path, then the designed concrete should be composed of small size aggregates and optimized mortar matrix.

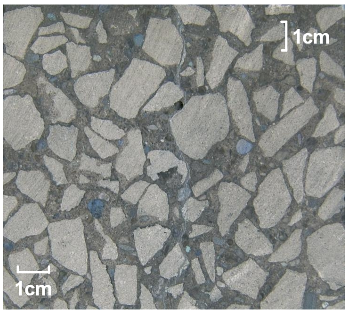

Figure 1. The micro-CT image of concrete meso-structure for numerical simulation

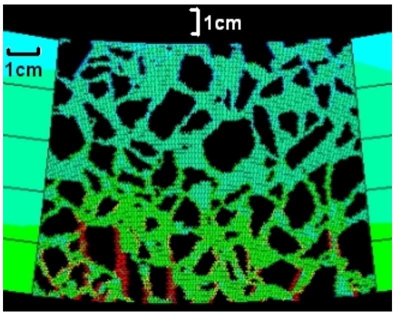

Figure 2. The predicted crack path denoted by red line on concrete meso-structure

4. OPTIMIZED MIX PROPORTIONS OF CONCRETE

Since the mix proportion of mortar should not be directly used for the concrete design, the mass fraction of each component is optimized according to the Chinese Standard “Specification for mix proportion design of ordinary concrete JGJ 55-2000”. The crushed basalt with particle size of 5 mm to 10 mm and the quartz with maximum size of 5 mm are used as the aggregates. The sand percentage（fine aggregate to total aggregate ratio by weight) is fixed as 0.38. The types and mass fractions of other components are unchanged with respect to those shown in Section 2.2.3. However, the sand-binder ratio is optimized to 1.5. Therefore, the optimized mix proportion of concrete is presented in Table 2. The curing system of concrete is the same as that of mortar. The primary mechanical properties of the designed concrete with hydration age of 28 days are listed in Table 3. As is shown in Table 3, although the elastic modulus and bending strength of the concrete are lower than the proposed values ($E = 30GPa, s_1 = 10MPa$), the compressive strength to bending strength ratio f_c / f_b = 5.84 is lower than that of a normal concrete with the similar compressive strength. It means that the toughness of the designed concrete is higher than that of the normal concrete.

Table 2. The optimized mix proportion design of concrete (unit: kg/m^3)

Cement	Fly ash	Aggregate		Latex powder	Defoaming agent	Water
		fine	coarse			
325	139	649	1059	13.9	1.4	176

Table 3. Primary mechanical properties of the designed concrete

Elastic modulus (GPa)	Poisson's ratio	Bending strength, f_b (MPa)	Compressive strength, f_c (MPa)	f_c / f_b
22.9	0.2	8.7	50.8	5.84

5. CONCLUSIONS

(1) By applying the multiscale material design theory, the primary material parameters are deduced for the meso- and micro-structure of the cementitious cover layer according to the proposed primary properties of the macrostructure. By means of such parameters, the reasonable mix proportion design of concrete is conducted by optimizing the parameters of the hardened cement paste and mortar matrix.

(2) The primary mechanical properties of the designed multiscale concrete structures are verified by laboratory mechanical tests. The modeling results show that the crack paths start from the mortar matrix, and extend along the boundary of coarse aggregates with large size. In other words, the coarse aggregates with large size are negative for the concrete toughening. Therefore, the concrete with high toughness should be designed using small size aggregates and flexible matrix.

(3) The prediction results and the test results show that the admixtures of the water dispersible latex powder and Class F fly ash are positive for the toughness of the designed cementitious cover layer.

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