Construction and Building Materials 127 (2016) 153–166

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat

Finite element-based micromechanical modeling of the influence of phase properties on the elastic response of cementitious mortars

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HIGHLIGHTS

- Microstructure-guided numerical simulation in cementitious composites.
- Stress distributions with varying inclusion stiffness and size distributions.
- Influence of matrix and interface stiffening/strengthening on composite response.
- Leads to material design strategies for non-conventional cementitious systems.

ARTICLE INFO

Article history:
Received 7 June 2016
Received in revised form 25 September 2016
Accepted 29 September 2016

Keywords:
Finite elements
Homogenization
Periodic boundary conditions
Microstructure
Constitutive behavior
Cementitious composite

ABSTRACT

This study reports the influence of inclusion stiffness and its distribution on the stress distributions in the microstructural phases of different cementitious mortars using microstructure-guided finite element simulations. Randomly generated periodic microstructures with single/multiple inclusion sizes and random spatial distribution, subjected to periodic boundary conditions and a strain-controlled virtual testing regime are chosen for final analysis. Numerical simulations reveal: (i) the differences in locations/magnitudes of stress concentrations as a function of inclusion stiffness and size distribution, and (ii) the sometimes detrimental influence of matrix and interface stiffening/strengthening on the overall composite response, leading to material design strategies when non-conventional inclusions are used in cementitious systems for special properties. The constitutive behavior in the linear elastic regime is extracted based on the predicted dominant principal stresses and strains in the representative area element. Thus, in addition to the microstructural phase stresses, this methodology also provides predictions of the composite elastic modulus, which are observed to be more reliable than those obtained from analytical prediction models.

1. Introduction

The link between the material microstructure and relevant mechanical properties provides valuable information towards design and development of sustainable cementitious materials for several applications. In recent years, many novel cementitious composites have emerged, incorporating several types of inclusion materials for various special applications such as the use of lightweight aggregates (LWAs) for internal curing, reduction of dead load, thermal and acoustic insulation [1–4], microencapsulated phase change materials (PCM) for control of thermal cracking in pavements and bridge decks [5] and regulating internal environment in buildings [6,7], waste and recycled materials such as rubber for energy absorption [8], and denser/stiffer aggregates for radiation shielding [9,10]. Incorporation of such inclusions influences the individual stresses in the microstructural components and the stress distributions in the composite, thereby dictating the failure path/mechanism of the material. Hence a comprehensive understanding of the influence of inclusion types on the microstructural stress distribution is necessary to design such materials for desired mechanical performance.

In an attempt to elucidate the influence of stiffness of inclusions on the distribution of stresses in the different phases in cementitious systems, this study employs a microstructure-guided micromechanical modeling scheme using the finite element method. Traditionally, the influences of inclusion type and stiffness on the mechanical behavior (elastic modulus, strength) of cementitious systems are evaluated experimentally [11–13], or through analytical approaches such as Mori-Tanaka [14–16] and double inclusion [17,18] models or iterative homogenization techniques [19,20]. Analytical homogenization techniques have been shown

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http://dx.doi.org/10.1016/j.conbuildmat.2016.09.153

to provide good estimates of the effective property of cementitious systems [21,22]. However, these analytical and semi-analytical homogenization techniques do not have the capability to evaluate local stress concentrations around inclusions which influence the macroscopic behavior, especially for cementitious systems that exhibit heterogeneity at a microscopic scale. Thus, microstructure-guided numerical modeling is a favored approach under such considerations. Microstructure-guided simulations have been performed on cementitious materials using randomly generated microstructures [23–28] or image-based microstructures [29,30]. A few recent studies have evaluated stress localization in the lightweight aggregate-matrix interface using an analytical approach [31] or through a macroscopic numerical simulation of a compression test [32], thus helping to understand the effect of soft inclusions on mechanical properties. In this paper, 2D periodic microstructures for mortars containing spherical quartz (stiff) or lightweight aggregate (soft) inclusions, including the interfacial transition zone (ITZ) around inclusions, are generated virtually and the representative element areas (REA) thus obtained are numerically analyzed using finite elements by invoking periodic boundary conditions [33–35]. The fundamental differences in stress distributions in the microstructure as a function of the inclusion type, and the relative efficiency of matrix and interface stiffening are clearly brought out. In addition, the constitutive relationships in the linear elastic regime (considering in-service performance of structures) are also evaluated for both the material systems considered. Such comprehensive numerical evaluations of fundamental differences in local micro-stress distributions imparted by differences in inclusion type, and its resultant influence on the macroscale mechanical response are rather uncommon.

2. Microstructural modeling

2.1. Phase elastic properties

The constitutive relationships for all the components: cement paste, hard (quartz aggregates) and soft (lightweight aggregate - LWA) inclusions, and the paste-inclusion interfaces are considered in their respective linear elastic regimes only. The default elastic properties of the components, extracted from available literature [14,36–41], are presented in Table 1. However, for parametric studies discussed later in the paper, a range of values are considered, which are indicated in the respective sections. The interfacial transition zone between cement paste and hard, non-porous aggregates such as quartz are known to be more porous than the bulk paste. In the case of saturated LWA inclusions in the mixture, they provide additional water and enables an increased degree of hydration, which densifies the microstructure. The densification is typically observed at the cement-aggregate interface [42], thereby stiffening the interface. This effect is accounted for in the parameters used for simulation.

2.2. Finite element models: examining the influence of boundary conditions and phase distribution

Two-dimensional plane strain microstructural finite element models are employed here in order to examine the influence of inclusion and matrix properties on the bulk elastic behavior of the composite system. A sufficiently large (4.15 mm × 4.15 mm) representative element area (REA) has been considered for the analysis. The spatial distribution of inclusions and the chosen boundary conditions play an important role in any numerical stress analysis procedure [33,34]. The choice of boundary conditions as well as the spatial distribution of inclusions need to be thoroughly investigated since the boundary conditions are applied on the REA and the averaged response of REA is used as an indicator of the influence of the microstructural phases. Hence, this section investigates the effect of different boundary conditions and distribution of inclusions (in the REA) on the stress distribution in order to establish the appropriate parameters for detailed studies. Under uniaxial conditions, the value of higher eigenstress is significantly higher as compared to the other two. Here, the values of σ_{11} and σ_{33} are always lower than σ_{22}. Hence, In this paper, dominant principal stress (σ_{22} in this case) is taken as the microstructural stress measure [32].

2.2.1. Regular arrays and essential boundary conditions

In many numerical stress analysis simulations of matrix-particulate inclusion composites (such as mortar or concrete), the actual material is simplified into a model that considers either a single spherical inclusion and the matrix surrounding it [43,44] or a uniform array of spherical (or circular, in 2D) particles in a continuous matrix [45,46]. The single inclusion case is generally applicable for low concentrations of particles (dilute limit). Fig. 1(a) shows a quarter model containing a uniform array of particles with essential (displacement) boundary conditions [47] applied at the left and bottom edges, considering symmetry. The REA contains circular quartz particles (aggregates) arranged in a square lattice within a cement paste matrix, and contains 50% inclusions. The interfacial zone around the aggregates are also accounted for. The top face of the geometry is subjected to uniform compressive loading parallel to the Y-axis. The analysis is performed using ABAQUS™. Fig. 1(b) shows the stress distribution in the REA for an applied external stress of 40 MPa. While this configuration results in concentration of stresses at the top face due to direct application of load, the stress concentrations at the left and bottom edges are avoided due to the effective clearance between the inclusions and the boundaries. Moreover, when considering a heterogeneous material such as cement mortar, such a perfectly ordered regular lattice structure of inclusions fails to capture the randomness of particle distribution and the resultant stress distributions. This limits the application of such models for the case of random particulate composites even when the assumption of homogeneity can be applied to the global microstructure.

2.2.2. Improvements through the use of periodic microstructure and periodic boundary conditions

The limitations discussed above necessitate improvements in the model formulation with respect to the geometrical features of the microstructure where the spatial randomness in particle distribution is considered. Fig. 2(a) shows such an improved model. The virtual random periodic microstructure is generated using a microstructural stochastic packing algorithm [48–50]. This algorithm requires the particle size distribution (PSD) and the volume fraction of particles as inputs and it packs the circular inclusions

Table 1
Elastic properties of the components of the mortar for FE simulations.

Elastic property	Hardened cement paste	Quartz inclusion	Quartz-cement paste interface	LWA inclusion	LWA- cement paste Interface
Young's Modulus, E (GPa)	20	70	15	16	30
Poisson's Ratio, υ (−)	0.22	0.17	0.22	0.20	0.20