Computational Materials Science 93 (2014) 29–35

Contents lists available at ScienceDirect

Computational Materials Science

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

Multiscale approach for the nonlinear behavior of cementitious composite

Rohit Raju Madke, Souvik Chakraborty *, Rajib Chowdhury

Department of Civil Engineering, Indian Institute of Technology Roorkee, Roorkee 247 667, India

ARTICLE INFO

Article history:
Received 23 April 2014
Received in revised form 11 June 2014
Accepted 16 June 2014

Keywords:
Polyurethane cement composite
Microstructure
Representative volume element
Mean field homogenization
Finite element analysis

ABSTRACT

This paper introduces a multiscale modeling approach to simulate the macromechanical properties of cementitious composites with polyurethane reinforcement. The polyurethane inclusions to hydrated cement paste matrix are represented by continuum 3D elements. Simulations of the real phenomenon that occur at the micro level of the composite have been done by mean-field homogenization technique and finite element analysis. The multiscale model presented in this work enables us to evaluate the stress–strain behavior and other engineering properties. Different configurations of polyurethane cement composite have been studied including variation of loading conditions, weight fraction of polyurethane and the aspect ratios of the polyurethane inclusion. The effect of shape and alignment of polyurethane on the stiffness of the composite has also been evaluated. Strength and stiffness values obtained from the proposed approach are in good agreement with that obtained from open literature.

1. Introduction

In recent days, cement–polymer composites are considered as one of the sustainable construction material in the construction industry [1,2]. These are obtained by partially replacing the cement hydrate binders with polymeric modifiers such as polymer dispersion, water soluble polymers, redispersible polymer powders, liquid resin, and monomers [3]. In 1923, Cresson first introduced the polymer–hydraulic cement system [4]. Compared to the conventional cement pastes, cement–polymer composites enhances compressive strength, flexural strength, tensile strength, adhesive properties, bearing capacity, good workability and reduces the quasi-brittle nature [5–7].

In general, following sequential operations are used to prepare cement polymer composite: (i) dry mixing of the powdered components thoroughly in a high intensity mixer, (ii) adding the liquid components, (iii) wet mixing to form a thoroughly blended mixture and (iv) then formed into any desired shape and cured. Other methods like impregnating the polymer into the cement paste by radiation polymerization techniques may also be used [8,9].

In this paper, we have developed a numerical model of two phase polyurethane cement composite (PUCC). The micro-mechanical properties of the phases are used to compute the macro-mechanical properties of the composite by considering a representative volume element (RVE) with periodic boundary conditions [10,11]. The macro-scale responses are calculated from the micro-scale responses, through a variety of methods, collectively referred to as mean-field (MF) homogenization [12] and/or by using finite element (FE) analysis [13]. At micro-scale, both polyurethane and cement matrix are represented by 3D continuum elements with three translational degrees of freedom. The bonding between the matrix and the inclusion is modeled with the aid of perfect interface model (stress approach) [14]. Furthermore, we have considered the inter-phase as a continuum material (same properties as the matrix), perfectly bonded [15,16] to the inclusion and to the matrix. The mesh of the interface does not share nodes with the mesh of the inclusions and the matrix. They are instead connected using tie constraints.

Schematic representation of the cementitious composites with polyurethane reinforcement is depicted in Fig. 1. In the present study, impact of aspect ratio, boundary conditions, different geometrical configurations (shape and sizes) on the composite are investigated. Furthermore, we have also introduced mean-field homogenization theory [17–19] to simulate in a compact form the macro-mechanical behavior of the cementitious composites, providing a further benchmark to the multiscale FE model of the cementitious composites. The FE code *ABAQUS*™ version 6.10 has been utilized for the numerical computations, due to the following reason: (i) The code is a well-known solver specifically developed for nonlinear simulations, (ii) The code is able to simulate complicated damage behavior in the structures, (iii) The finite

* Corresponding author. Tel.: +91 9720450402.
E-mail address: csouvik41@gmail.com (S. Chakraborty).

http://dx.doi.org/10.1016/j.commatsci.2014.06.026
0927-0256/

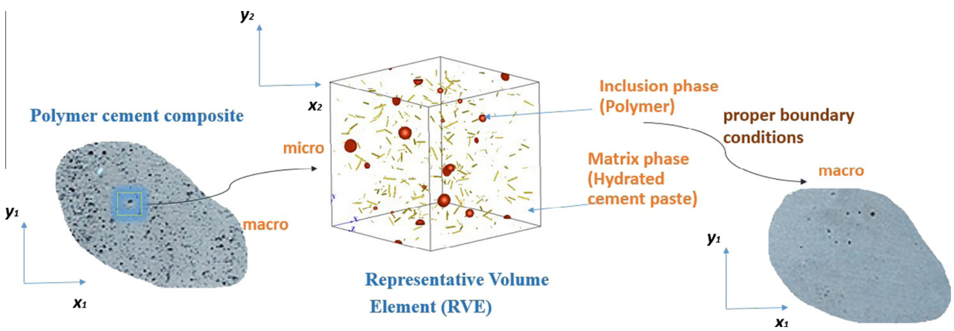

Fig. 1. Macro–micro-macro transition for a composite material reinforced with multiple phases of inclusions.

element based tool offers python language based scripting and subroutines, which is very useful in simulating debonding of interphase.

2. Multiscale analysis

A direct numerical simulation of microstructures is needed to establish an exact representation of the heterogeneous structure that appends and contains all the details at the micro scale. But in order to extract all the details, it will lead extremely fine spatial discretization with a very large meshes of finite elements to carry the information at the microscale which is computationally very expensive. Realistic representation of heterogeneous materials can be obtained by so called RVE [10,20,21]. An RVE is a small micro sample that contains a finite part of the inclusions and matrix that represents an idealization of the actual microstructure of the composite. RVE in combination with proper boundary conditions represent the material macro behavior as close as possible.

The concept of homogenization was formulated by Sequet in 1987 [22]. For heterogeneous materials like cement polymer composites, constitutive equations for microscopic properties can be determined by specifying the RVE, localization and homogenization details. For localization, the microscopic boundary conditions (BC) are determined from the macroscopic BC based on geometry and the constitutive laws. Homogenization is the determination of macroscopic properties based on the analysis of RVE. However, homogenization can be applied if and only if two length scales can be defined [22]. In the framework of the mean field theory, macro fields can be defined as the [weighted] averages of corresponding micro fields. The effective properties are expressed in terms of averaged micro fields. For any two phase composite, the volume average of the strain field over the RVE can be given by

$$\langle\varepsilon\rangle_w = v_m\langle\varepsilon\rangle_{w_m} + v_i\langle\varepsilon\rangle_{w_i} \tag{1}$$

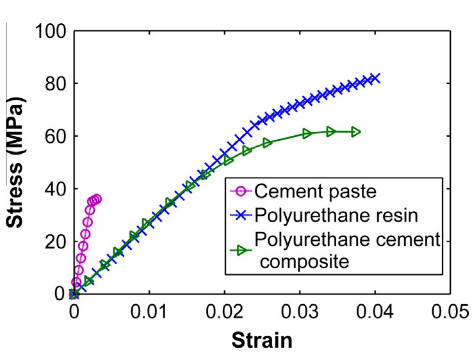

Fig. 2a. Stress–strain behavior for hydrated cement paste [30], polyurethane resin [35], and resultant composite [40].

where $\langle\varepsilon\rangle_w$ is the strain field, v is the volume fraction, m denotes matrix and i denotes inclusion. Eq. (1) is applicable for any micro-field, for example stress field. MF model can be defined by using strain concentration tensors A and B such that

$$\langle\varepsilon\rangle_{w_i} = A\langle\varepsilon\rangle_w;\ \ \langle\varepsilon\rangle_{w_i} = B\langle\varepsilon\rangle_{w_m} \tag{2}$$

First order Mori–Tanaka homogenization scheme for MF has been selected for this study. Mori–Tanaka method was proposed by Mori and Tanaka in the year 1973 [17–19]. This method is based on Eshelby's elasticity solution [17,23]. According to Eshelby, for a homogeneous isotropic infinite body with an ellipsoidal inclusion subjected to a uniform eigenstrain E, the resulting strain field within the inclusion is uniform and can be given by

$$\langle\varepsilon\rangle_w = \xi - E \tag{3}$$

where ξ is the fourth rank Eshelby tensor and depends upon the geometry of the ellipsoidal inclusion and Poisson's ratio [23–25]. Considering C and S as the uniform stiffness and compliance for corresponding phases, the relation between the average composite strain and the average inclusion strain can be given by

$$\begin{aligned}\langle\varepsilon\rangle_w &= \langle\varepsilon\rangle_{w_i}[I + \xi S^m(C^i - C^m)]\\ \langle\varepsilon\rangle_{w_i} &= A^{\mathrm{Eshelby}}\langle\varepsilon\rangle_{w_i}\end{aligned} \tag{4}$$

Each inclusion in the RVE behaves as if it were isolated to the real matrix. Mori–Tanaka's assumption is that the far field (remote) strain observed in each single inclusion is equal to the average strain of the matrix rather than the composite as in the Eshelby's case.

$$\langle\varepsilon\rangle_{w_i} = A^{\mathrm{Eshelby}}\langle\varepsilon\rangle_{w_m} \tag{5}$$

In order to generalize the MF scheme from linear elasticity to nonlinear regime, linearization has been done by the incremental method [17,26]. Using the above equations, the effective average strain field values for the composite have been computed. Similar to the strain field, other micro fields can be found by these formulations. In order to predict the constitutive behavior of the heterogeneous material and interaction between the overall effective properties between the macrostructure and the microstructure, the different phases of the material need to be modeled for microstructural information and simulation data. The matrix phase consists of hydrated cement paste whereas the inclusion phase

Table 1
Mechanical properties of each material.

Property (units)	Hydrated cement paste	Polyurethane resin
Density (kg/m^3)	2000	400
Young's modulus (GPa)	15.2	2.67
Poisson's ratio	0.24	0.30–0.50 [40,41]