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Multiscale modeling of carbon nanotube reinforced concrete

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ABSTRACT

The present paper proposes a hierarchical multiscale approach in order to evaluate the nonlinear constitutive behavior of concrete reinforced with carbon nanotubes (CNTs). To this purpose, representative volume elements, consistent to the microstructural topology of the material, are constructed and analyzed using finite elements. As the dimensions of the CNTs and those of a typical mesoscale concrete RVE differ by orders of magnitude, a hierarchical multiscale analysis strategy is implemented to pass information through scales with different RVEs assigned at each scale of separation. Both elastic and inelastic analyses are performed on all scales for various CNT weight fractions, defining a different nonlinear constitutive stress–strain behavior at each scale of separation. It is shown that the proposed computational approach can be used alternatively to corresponding costly experiments in order to accurately evaluate the nonlinear constitutive behavior of such complex materials.

1. Introduction

The investigation of the complex behavior of concrete requires its description as a composite material with randomly defined microstructural topology. The aggregates generally occupy 60%–80% of concrete and significantly affect its mechanical properties. The sand, the gravel and the crushed stones are the main aggregates. The separation for the sand and gravel is usually made for diameters of 4.75 mm. The shape and properties of the aggregates and the cement paste depends mainly on their type [1–16]. The gravel, in general, have a rounded shape while the crushed stones are more angular. The so-called aggregate concrete curves characterize the cumulative distribution of aggregates in concrete, usually expressed as cumulative percentage of aggregates that cross a specific sieve. One of the most used family of such curves are the Fuller diagrams which depict the distribution of aggregates, whose curve lies within the permitted limits A32, B32 of the German code DIN 1045. In practice, concrete is usually constructed based on the Fuller curves, which leads to optimal distribution of density and strength of concrete [17–22].

In order to upgrade concrete performance, effort has been put in improving the cement paste mechanical properties by adding fiber reinforcement such as glass or steel fibrils [22–25], while recently nanoscale inclusions, such as CNTs, were added [16,26,27]. The results in the latest case were encouraging since the improvement of the mechanical behavior of cement paste ranged in percentages from 13% to 17%, even for a small weight fraction of less than 2.00%. Makar et al. [26] experimented with three different samples of cement paste. The first had a water to cement factor equal to 0.80 while the remaining two of 0.50 and 0.40, respectively. The percentage of added carbon nanotubes approached the value of 2.00% by weight. In this work, the measurements were made as a function of hydration of the cement paste and it was observed that hydration of the cement paste results in reversing the positive effects of carbon nanotubes.

Although CNT-reinforced concrete is material with exponentially increasing interest, very few works on its modeling have appeared over the past years. Most of these works are restricted to the modeling of cement paste reinforced with CNTs [28,29]. In these works homogenization methods or micromechanics approaches are used. On the other hand, multiscale strategy of neat concrete has attained considerably attention by detailed modeling of aggregates and extraction of homogenized compressive and tensile nonlinear constitutive behavior [30,31] or other concrete parameters [32,33]. In the abovementioned approaches, the basic ingredients of computational multiscale analysis have been applied in the same manner as in more classical composite material applications such as CNT-reinforced polymers [34–52]. Nevertheless, there is a great shortage in the successful modeling of concrete, especially with carbon nanotubes reinforcement. Remarkable literature [32,33,53–55] concentrates on the computational simulation of cement paste or reinforced concrete or is far from the quick, efficient and flexible simulation of neat concrete. It often does not distinguish between cement paste and aggregates and prevent the designer to experiment with more concrete compositional choices. At the same time, the literature on carbon nanotube reinforced concrete [56–59] proposing cumbersome models requiring immense computational power

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(e.g. molecular dynamics) or techniques that cannot result in a total design of carbon nanotube reinforced concrete from its cement paste's analyses. The main advantage of this computational approach is the efficiency and the flexibility in design in each separate scale where the contribution of each scale amplifier is highlighted using computationally affordable techniques.

The present work proposes a hierarchical multiscale computational methodology in order to evaluate the nonlinear constitutive behavior of concrete reinforced with carbon nanotubes (CNTs). To this purpose, RVE specimens are numerically constructed in a consistent to the microstructural topology of the material manner and analyzed subsequently using finite elements in order to extract homogenized equivalent material properties. As the dimensions of the CNTs and those of a typical mesoscale concrete RVE differ by orders of magnitude, a hierarchical multiscale analysis strategy is implemented to pass information through different scales. The RVE dimensions for each scale of separation are the following: (a) a cube of dimensions (1200^3 nm^3) consisted of only cement paste and CNTs, and nano-to-mesoscale RVEs with dimensions (b) 10^3 mm^3 (RVE 2), (c) 40^3 mm^3 (RVE 3) and (d) 150^3 mm^3 (RVE 4) for each size class of aggregates, respectively. The size class of aggregate depends on the category of the sieve that is crossed. This model separation, with respect to the aggregate size, is necessary in order to avoid complicated and very refined finite element meshes that lead to computational intractability. For the shake of simplicity, all aggregates are assumed spherical in shape. Both CNTs and aggregates inclusions are considered fully bonded with the surrounding cement paste and modeled using the embedded finite element technique. Both elastic and inelastic analyses are performed on all scales, defining a different damage model at each scale. Sensitivity analysis is carried out with respect to CNTs weight fraction (wf). The nonlinear constitutive stress–strain behavior is computed at each scale, for the various CNT wfs considered. From these analyses it is found that the improvement of the concrete mechanical behavior ranges from a 5% to 12% increase in peak compressive strength depending on the CNTs wf, while the tensile stress behavior remains almost insensitive to the addition of CNTs. Furthermore, it is shown that proposed computational multiscale analysis approach can accurately and efficiently predict the behavior of composite materials with complex microstructures, and can be used alternatively to corresponding costly experiments.

The above methodology is clearly not limited to carbon nanotube reinforcement but can be easily implemented in any other application of concrete reinforced with nanoscale or mesoscale materials. Once again, the hierarchical analysis from nanoscale to the mesoscale is considered ideal, and in combination with alternative theoretical approaches to existing literature [67,70] leads to the efficient modeling of the concrete behavior and of other mechanical properties, which is not mentioned here. Furthermore, if the hypothetical problem requires too much accuracy in the detail (bond failure, fiber sliding) there are great existing methodologies [68] for efficient and quick modeling with affordable computational cost while in parallel it is possible to include stochastic parameters on the nanoscale for a holistic design [69,71–73] without damaging the effectiveness of this methodology. Consequently, this technique, combined with existing theoretical approaches, can simulate every concrete characteristic from nanoscale to mesoscale.

2. Hierarchical multiscale modeling strategy

In this work, a hierarchical multiscale modeling strategy is implemented in order to model mesoscale RVE specimens of concrete reinforced with CNTs. To this purpose, the target mesoscale concrete RVE specimen of Fig. 1 is considered which contains all reinforcing elements, i.e. aggregates of all dimension (from 0.125 mm to 32 mm), as well as CNTs at a lower nanoscale. A detailed model with accurate resolution in all scales of this RVE is practically impossible, therefore, hierarchical steps are implemented in which the target RVE of Fig. 1 is

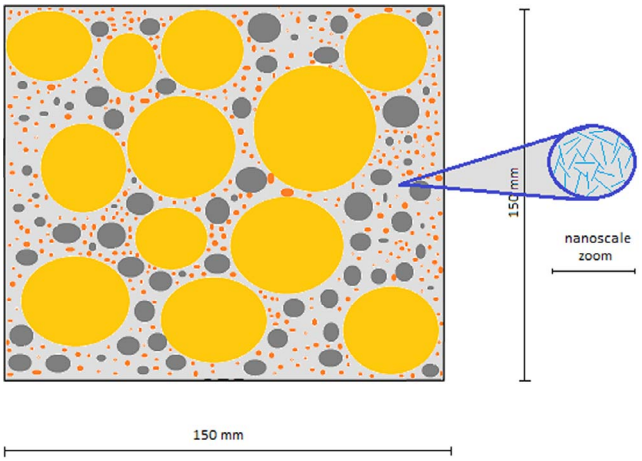

Fig. 1. Target concrete mesoscale RVE with various size of aggregates and zoom at nanoscale CNT reinforcement.

broken down in RVEs of lower dimensions, as shown in Fig. 2. Initially resolved, the lowest nanoscale RVE 1 contains only the cement paste and carbon nanotubes (Fig. 2(a)). Computational homogenization on RVE 1 leads to an equivalent “enhanced” cement paste called cement paste 2. Then, using this new cement paste 2, an upscale RVE containing aggregates up to 2 mm is constructed (Fig. 2(b)). Subsequently, a new RVE is obtained containing aggregates up to 8 mm and a further enhanced cement paste (cement paste 3). Finally, the last RVE is constructed at the mesoscale dimensions, containing aggregates up to 32 mm diameter and an even more enhanced cement paste 4. This model is considered to be equivalent to a hypothetical detailed model of the target specimen of Fig. 1.

2.1. Modeling of RVE 1

RVE 1 (Fig. 2(a)) consists of only CNTs embedded in a surrounding cement paste. Following the steps described in [45], the RVE 1 model is constructed following a sequential approach as shown in Fig. 3. At the lowest scale, the interatomic relations between carbon atoms are governed by a quadratic force field potential and a molecular structural mechanics (MSM) model is formed for the simulation of stand-alone CNTs. According to MSM, the C–C covalent bonds are substituted by continuum beam elements allowing the atomic lattice of the nanotube to be modeled as a nanoscale space frame. Proceeding to the next scale, the space frame is reduced to an equivalent beam element (EBE) which is used as the basic structural element in the chain construction of long microscale CNT “ropes” inside the surrounding matrix. The final microstructured RVE model is formulated by embedding these equivalent beam elements into the finite element discretized bulk matrix. A detailed description of the MSM approach as well as the multiscale modeling steps followed for the discretization of a microstructured RVE model with only one CNT, is given in detail in [45–48].

The molecular structural mechanics approach and its modified version (mMSM) used here, belongs to the equivalent continuum modeling (ECM) approaches which tend to be a more efficient modeling strategy for simulating larger scale systems and longer time spans compared to ab initio or other molecular dynamics (MD) simulations. The core principle in these methods is to establish a linkage between molecular and structural mechanics, based on systems energy equivalence developed due to chemical bonds between carbon–carbon atoms (C–C) and the strain energy of a solid beam element following by continuum mechanics. Thus, having adopted a quadratic potential force field to account for linear covalent C–C interactions and a rectangular beam element in the context of finite element method, the following relationships between structural mechanics parameters and molecular mechanics force field constants are derived: