Construction and Building Materials 50 (2014) 317–327

Contents lists available at ScienceDirect

Construction and Building Materials

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

A multi-scale approach for evaluating the mechanical characteristics of carbon nanotube incorporated cementitious composites

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HIGHLIGHTS

- Multiscale approach for evaluation of properties of CNT incorporated cement paste.
- Unified expression to determine the properties of CNT using interatomic potentials.
- Proposal for evaluating response at microlevel using representative volume element.
- Evaluation of macro-level response of elements with CNT modified cement composite.

ARTICLE INFO

Article history:
Received 11 April 2013
Received in revised form 18 September 2013
Accepted 24 September 2013
Available online 17 October 2013

Keywords:
Nano filament
Carbon nanotube
Young's modulus
RVE
Cementitious composite
Strength
Non-linear analysis
Different scales

ABSTRACT

Cementitious composites are limited to the applications due to their lesser tensile strength and strain capacity. In the present study, an attempt has been made to improve the properties of cementitious composites using nano filament like materials such as carbon nano tube (CNT). Since, there is no well-established technique to determine the engineering properties of CNT of various geometries which is essential for effective application of the same to cementitious composite, a unified approach has been proposed by combining the classical and numerical method. Further, a square RVE of CNT incorporated cement paste is developed in which CNT is simulated as an equivalent continuum model at micro-level. The effect of variation of the percentage of CNT in the cementitious matrix on the strength and stiffness of CNT incorporated cement matrix is evaluated. Finally, with the evaluated properties of CNT reinforced cement both at nano and micro-level, non-linear FE investigation has been carried out to evaluate the macro response of structural component with varied degree and disposition of CNT incorporated composite. The findings of the present study will provide insight into the newly emerged material and its alluring scopes for application as construction and building materials.

1. Introduction

Cement, the most extensively used construction material, has very less tensile strength and ultimate strain capacity. Research is being carried out over the years for improving its properties by addition of fibers (macro to micro). Nano-modification of cement is an emerging field. Cement can be nano-engineered by incorporation of nanosized building blocks (e.g., nanoparticles and nanotubes) to control material behavior and add novel properties, or by the grafting of molecules onto cement particles, cement phases. Much of the work to date with nanoparticles has been done with nano-silica (nano-SiO_2) and nano-titanium oxide (nano-TiO_2). There are a few studies on incorporating nano-iron oxide (nano-Fe_2O_3), nano-aluminum oxide (nano-Al_2O_3), and nanoclay particles [1]. Recently, exceptional types of carbon nanofilaments have raised the interest of some concrete researchers because of their remarkable mechanical, chemical, electrical, and thermal properties, and excellent performance in reinforcing polymer-based materials [2–4]. Nano-reinforcements delay the nucleation and growth of cracks at the nanoscale and stop their propagation to the micro-level. These nanofilaments, both Carbon Nanotubes (CNTs) and Carbon Nanofibers (CNFs), may prove to be the promising candidates for the next generation of high-performance and multifunctional cement-based materials and structures.

CNT is a cylindrical nanostructure which could be thought of formed by rolling of a graphene sheet. There are two common types of nanotubes based on the way the graphene sheet is rolled to form CNT; they are zigzag and armchair. The radius of the nanotube ranges from 0.3 nm to 1000 nm and has a very high aspect

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http://dx.doi.org/10.1016/j.conbuildmat.2013.09.053

ratio. CNT may be single walled or multiwalled. Single Walled Nanotube (SWNT) is a single sheet of graphene rolled into a cylinder and Multi Walled Nanotube (MWNT) has many layers of graphene sheet rolled coaxially around a hollow core.

Since the discovery of CNT by Iijima [5], it is being used in various applications ranging from nanoscale electronics to filler materials in paints and plastic composites. But, its potential application in construction industry has not been fully explored. Also, the mechanical properties of CNT and its composite action when dispersed with other materials are not completely understood.

The research on CNTs and composites are going on in wide range of length scales. A group of researchers are working onto determine the Young's modulus of CNT (nanoscale) using experimental methods like High Resolution Transmission Electron Microscopy (HRTEM) ([6], Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) [7] and theoretical methods like Molecular Dynamics [8,9], Continuum Mechanics [10] and Finite Element Analysis [11,12]. Other group of researchers are working at Representative Volume Element (RVE) (microscale) to study the interaction of CNT and the surrounding matrix like the load-transfer behavior and to evaluate the effective material properties of the composite material under different loading conditions [13–15]. Yet another group of researchers are working onto determine the mechanical properties of structural elements reinforced with CNTs (macroscale) subjected to different loading conditions [16–18].

There are also few experimental investigations in which the researchers vary the percentage of CNT and the dispersion mechanism and determine the improvement in the mechanical properties of the material. Konsta-Gdoutos et al. [17] experimentally investigated the reinforcing mechanism of MWNT in cement based materials by incorporating CNTs of 0.048% and 0.08% of weight of cement. Sanjeev kumar et al. [18] added CNTs of 0.5%, 0.75% and 1.0% in cement and evaluated its compressive and tensile strength. It is further observed that the results reported from the experimental investigations are not always consistent. When Abu Al-Rub et al. [19] reported the increase in percentage of flexural strength to 269% by incorporating 0.2% of CNT from their experimental studies; Luo et al. [20] reported only 35.4% increase in percentage of flexural strength for the same percentage of CNT. Similar type of contradictory results from experimental investigations has also been reported by researchers by adding up to 1.5% of CNT into the matrix. Hence, an intensive study has to be carried out to evaluate the effect of percentage of CNT on the mechanical properties of CNT incorporated composites.

In recent years, computational investigations are going on all over the world for evaluating the mechanical properties of CNTs and CNT reinforced composites; both to explain the observations and to obtain information that are not accessible through experiments. Also it helps in providing some initial guidelines to the experimental works which will help to minimize the scope, cost and time for the experiments. CNT composites can be modeled using two basic methods – discrete and continuum methods. In discrete methods such as Molecular Dynamics (MDs), atoms are modeled as individual particles and potential theories are applied to calculate the forces among these atoms. These methods are applicable to small length scales and cannot deal with larger length scales. In engineering applications, nanocomposites extend from nano to micro or even to macro scale which is difficult to address using MD method and hence some other simulation techniques should be used separately or with MD to address these kinds of problems. Continuum mechanics approach can be used for this purpose. But while using continuum mechanics approach, every attempt should be made to check if all the assumptions of continuum mechanics hold good for nanomaterials. Also, in order to bring the scientific advancement to engineering applications, it is utmost important to establish the link between the findings and outcome from the research in varied scales and aspects.

In this study, the behavior of the material in different length scales is investigated and tried to take forward the properties from one scale to the other. A unified approach combining the nanoscale continuum theory and numerical simulation has been proposed to determine the tensile stiffness (and thus the Young's modulus) of the CNT which considers the interatomic potential between atoms and also the geometric parameters like chirality and radius. The Young's modulus of CNT, as observed from the study is used to model the Representative Volume Element of CNT reinforced hydrated cement paste. (Hereinafter "hydrated cement paste" will be referred as "cement"). Expressions derived from strength of materials approach are used to determine the mechanical properties of the RVE subjected to axial stretch. The effect of various parameters like percentage of CNT and arrangement of CNTs in cement matrix on the strength and stiffness of CNT reinforced cement is also investigated. With the evaluated properties of CNT reinforced cement paste from RVE, an investigation has been carried out on the behavior of a composite beam reinforced with different percentages of CNT and by varying the depth of composite layer. The present study and its findings will be helpful towards developing new cementitious materials with enhanced engineering properties.

2. Tensile stiffness of carbon nanotubes

The Young's modulus and therefore the tensile stiffness of CNT is still a paradox and an appropriate method is needed for evaluating the same so that it can be effectively utilized in composites. It is difficult to conduct experiments and to establish atomistic studies at nanoscale. Hence, a simplified mathematical model is developed to determine Young's modulus of CNT of armchair and zigzag tubes using nanoscale continuum theory developed by Zhang et al. [21] and a numerical model developed by Jalalahmadi and Naghdabadi [22]. The effect of various parameters like chirality, tube radius and aspect ratio on the Young's modulus of CNT was also observed and a simplified expression is proposed for determining the same.

Zhang et al. [21] proposed nanoscale continuum theory using interatomic potential by which the tensile stiffness of SWNT is given by,

$$E_{inter} = C_{ZZZZ} \frac{C_{ZZZZ}^2}{C_{\theta\theta\theta\theta}} \tag{1}$$

where Z is the axial direction and θ denotes the circumferential direction of SWNT.

The linear elastic tensile stiffness as obtained above does not depend upon its geometry. In order to find out the dependence of Young's modulus of SWNT on its geometrical parameters like chirality, tube radius and the aspect ratio, an investigation has been carried out using numerical simulation.

2.1. Material properties and analysis method adopted

A 3-D Finite Element Model was developed in ANSYS in which nodes were placed in the location of carbon atoms and the covalent bonds between the carbon atoms were replaced by three dimensional BEAM 4 elements. BEAM4 element has six degrees of freedom and is defined by two nodes as well as its cross-sectional area, two moments of inertia, two dimensions and material properties. In the present study, circular cross-section with a diameter of 0.1296 nm was adopted for the beam elements and the material was considered to be linear and elastic with the Young's modulus of 9.382 TPa and the Poisson's ratio of 0.3, as adopted by Jalalahmadi and Naghdabadi [22].