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Multiscale dynamic fracture behavior of the carbon nanotube reinforced concrete under impact loading

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ABSTRACT

In this paper, the impact behavior of the carbon nanotube reinforced concrete is investigated through the multiscale simulation. At the nano scale, properties of carbon nanotubes are determined through the molecular dynamics simulation. Afterwards, a finite element based hydration model of the cement is adopted to disperse the CNTs on the surface of the cement. At the meso scale, the concrete is simulated by considering all three phases including, cement, aggregates and interfacial transition zone (ITZ), to obtain a homogenized response. Finally, at the macro scale, the homogenized response is used to find the behavior of CNT-reinforced concrete under impact loading. The results indicate that less damaged areas are generated in the CNT-reinforced concrete model. It responses with higher resistance and energy absorption capacity, which results in considerable reduction of the penetration depth to contain a projectile.

1. Introduction

Nowadays, an increasing demand has generated for the production of high-performance engineering materials with outstanding mechanical properties for better protection of structures against extreme loadings such as impact and blast. The dynamic behavior of structures have further been brought to forefront of civil engineering research after catastrophes such as Oklahoma City bombing and the September 11. Hence, construction of structures and buildings with high performance materials against such phenomena is essential. Researchers try to probe deeper into designing high-strength structures to sustain extreme loadings. A reliable design of concrete structures depends significantly on the understanding of its dynamics properties. Therefore, realizing the response of concrete structures subjected to high strain rate explosive loadings becomes inevitable as the behavior of the concrete subjected to impact loading differs from the static loading due to the strain rate effects.

The major weakness of the cement is attributed to its weak strength and rapid crack growth in tension. Due to the brittle nature of the concrete, researchers have tried to improve its resistance and performance under explosive and impact loading through several methods such as addition of various types of fiber to the concrete (FRC). Several types of fiber can be implemented into the concrete such as steel, polypropylene and carbon fibers. They can increase ductility, fracture energy, mechanical strength and resistance against impact loadings and also prevent the crack propagation in the concrete.

Recently, several authors have studied the impact behavior of fiber-reinforced concretes. Among them are Sovják et al. [1] who investigated the effects of impact loading on the response of Ultra-High Performance Fiber Reinforced Concrete (UHPFRC) slabs. Their results indicated that the optimal volume fraction of the fibers were 2% and using more than 2% did not improve the damage behavior. In addition, the dynamic impact behavior of the steel fiber reinforced concrete (SFRC) at different strain rates was studied by Xu et al. [2,3]. They illustrated that addition of fibers increased the stress and strain redistributions and the ductility of the sample. The SFRCs showed much enhanced crack-bridging effect at higher strain rates. Alavi Nia et al. [4] investigated the effects of different volume fractions of fibers on the impact behavior of fiber reinforced concrete (FRC). Their results indicated that fibers could increase the impact resistance of concrete specimen. They found that effect of fibers was more obvious in normal strength concrete than high-strength concrete and also steel fibers were more effective than polypropylene one. The studies of Nyström et al. [5] showed that the crack

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propagation and the penetration depth resistances of the fiber-reinforced concrete against projectile were improved and so they could be efficiently used in the protective structures.

A novel type of reinforcement for polymers, composites and also concrete is the carbon nanotube (CNT) [6], which is a very high strength material at the atomic scale. CNTs are hollow cylindrical structures made of carbon atoms at the nano scale. Its strength is more than a hundred time of steel and its elastic modulus is in the range of a Terapascal. Recently, several authors have studied the mechanical and engineering properties of the CNTs [7–9]. More details about these researches can be found in Ref. [10]. Inclusion of CNTs can improve the post-cracking behavior of the concrete material and consequently, CNT-reinforced concrete is expected to be a good candidate for blast-resistance structures by decreasing the penetration depth and damage of the structure.

In order to study the impact response of such material, it is essential to analyze the behavior of components of the concrete, and their collective response more accurately. Unfortunately, classical continuum theories cannot predict such complex behavior and more advanced methods should be adopted. Recently, several advanced computational methods such as meshfree [11–15] and multiscale methods were developed for fracture analysis [16,17] and crack propagation [18,19] in homogenous and heterogeneous materials. They estimated the material properties at the finer scales and used them as input parameters for the coarser one.

Moreover, several authors have studied the multiscale simulation of CNT-reinforced composites [20–22]. In a recent study, Eftekhari et al. [10] studied the quasi-static crack propagation of CNT-reinforced cements by the extended finite element method. Their results indicated that addition of CNTs to the cement paste, significantly increases the fracture energy and tensile strength of CNT-reinforced cement in static and quasi-static solutions. Furthermore, they illustrated that longer CNTs could increase the mechanical properties more than the shorter ones. In this research, the same methodology is further extended to investigate the effects of CNTs on the mechanical and impact behavior of the CNT-reinforced concrete using an advanced multiscale method. The physics of the model is extended to dynamic impact analysis and the effects of penetration of projectile and contact between the target and the projectile are considered.

Hence, at the atomic level, the mechanical properties of CNTs are investigated through the molecular dynamics simulation. Afterwards, at the micro scale, the mechanical properties of CNTs are incorporated in a finite element based cement hydration model to extract the mechanical properties of the CNT-reinforced cement. Then, at the meso scale, the concrete is modeled as a three-phase material, consisting of aggregates, cement paste reinforced by CNTs and interfacial transition zone (ITZ) which surrounds the aggregates. Finally, at the macro level, the effects of a projectile on the CNT-reinforced concrete specimen is investigated through the finite element simulation. A schematic representation of the mentioned procedure is depicted in Fig. 1.

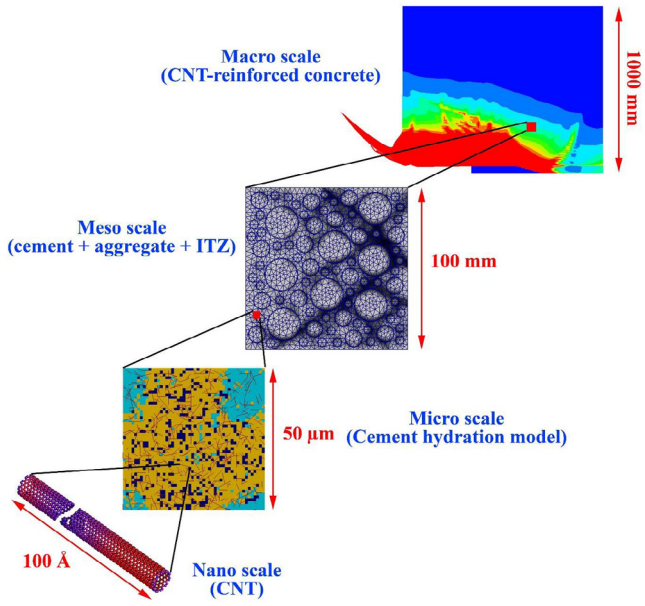

Fig. 1. Schematic representation for the dynamic multiscale simulation of impact and penetration of a projectile into a CNT-reinforced concrete.

2. Nano scale

First, the molecular structure of CNT is accurately simulated by the molecular dynamics (MD) approach. The LAMMPS (Large-scale atomic/molecular massively parallel simulator) open source code [23] is adopted to perform the MD simulations of CNTs under tensile and compressive loadings and to obtain the corresponding stress–strain curves.

In real applications, different types of CNTs may be created during the production and mixture processes. A chiral vector (n,m) defines the atomic configuration of the CNT structure. When n is equal to m, the CNT is called armchair and in the case of m equal to zero, it is called zigzag CNT. A CNT with a single tube is called single-walled CNT (SWCNT) whereas a multi-walled CNT (MWCNT) consists of several coaxial SWCNTs with an interlayer spacing of 0.34 nm. Two types of SWCNTs (diameter equal to 13.31 Å) and MWCNTs (diameter equal to 20.34 Å) with the length of 100 Å are considered in this study. SWCNTs and MWCNTs consist of 1650 and 4100 atoms, respectively.

To describe the interatomic interaction among the carbon atoms, the Tersoff potential function [24] is employed. In the Tersoff potential, the total potential energy of an atomic system is described as:

$$E_{ij}^{Tersoff} = \frac{1}{2} f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{1}$$

$$f_R(r_{ij}) = A_{ij} exp(-\lambda_{ij} r_{ij}), \quad f_A(r_{ij}) = -B_{ij} exp(-\mu_{ij} r_{ij}) \tag{2}$$

$$f_C(r_{ij}) = \begin{cases} 1, & r_{ij} \le R_{ij} \\ \frac{1}{2} + \frac{1}{2} cos\left[\pi (r_{ij} - R_{ij})/(S_{ij} - R_{ij})\right], & R_{ij} < r_{ij} < S_{ij} \\ 0, & r_{ij} \ge S_{ij} \end{cases} \tag{3}$$

where $f_R(r_{ij})$, $f_A(r_{ij})$ and $f_C(r_{ij})$ are the repulsive, attractive and cut-off functions, respectively, and r_{ij} is the interatomic distance between

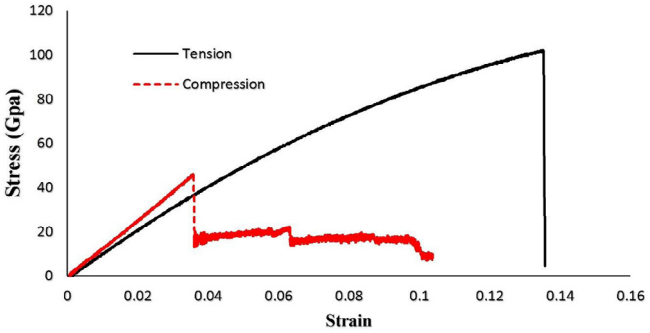

Fig. 2. Stress–strain curve for CNTs.