FINITE ELEMENT SIMULATION OF NANO-FILAMENTS PULL-OUT FROM CEMENTITIOUS NANOCOMPOSITE MATERIALS USING AN ELASTIC-PLASTIC-DAMAGE AND COHESIVE SURFACE MODELS

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Abstract

The main focus of this work is on investigating computationally the pull-out behavior of nano-filaments from the cement matrix. The effects of: (1) nano-filament-cement interfacial shear strength, stiffness, and fracture energy; (2) the mechanical properties of the cement; and (3) nano-filament mechanical properties, aspect ratio, and surface area to volume ratio on the pull-out strength from a cement matrix are investigated through simulating the nano-filament pull-out. A coupled elastic-plastic-damage constitutive model is adopted to simulate the behavior of the cement matrix, whereas the continuum shell model is used to simulate the elastic behavior of the nano-filament. The surface-based cohesive behavior is employed for modeling the interface between nano-filament and cement matrix. It is shown that the nano-filament pull-out force is mainly governed by the interfacial fracture energy, and not the interfacial shear strength. It is also shown that the pull-out strength and damage evolution in the cement matrix during the pull-out process are independent of the nano-filament embedded length, while the final debonding displacement is increased with the increase of the embedded length. Finally, it is shown that the Young's modulus and surface area to volume ratio of the nano-filament are other important key parameters that alters the pull-out strength.

1. Introduction

Carbon nano-filaments such as carbon nanotubes (CNTs) and carbon nanofibers (CNFs) have recently been integrated in the most widely used material in the world "concrete" for improving its mechanical properties and fracture resistance. However, such integration has led to marginal improvements due to the lack of fundamental understanding of the key factors that control the dispersions and interfacial bond of CNTs/CNFs with the cement matrix. The focus of this study is on the second issue of studying the effect of CNT-cement interfacial properties on two main properties; the CNT's pull-out force, which greatly affects stiffness and strength of the nanocomposite cement, and the total CNT's debonding displacement, which greatly affects the ductility of the nanocomposite cement. Therefore, the CNT pull-out behavior from the cement matrix has a controlling effect on the overall stiffness, strength, and fracture toughness of CNT/cement composites. If micro-cracks to be bridged successfully by CNTs in order to effectively suppress their propagation, then the CNT/cement interface should be engineered to control this bridging behavior and consequently enhance the overall (macroscopic) mechanical properties of the CNT/cement composite.

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Due to the difficulty in experimentally investigating the interfacial properties, bond, and pull-out of a single CNT within a matrix material [1], accurate computational modeling is greatly needed. To the authors' best knowledge, unlike CNT/polymer composites [2], no experimental attempt has been made until now to directly investigate the pull-out behavior of a single CNT from the cement matrix. Therefore, one can argue that simulating the single CNT pull-out from the cement matrix might be very useful in providing considerable insight into the load transfer mechanism between the cement matrix and the CNT, and how to control the global mechanical properties of the CNT-based composite.

This paper focuses on investigating the role of the interfacial properties (namely, stiffness, cohesive shear strength, cohesive energy), CNT's elastic modulus, CNT's size and aspect ratio, CNT's embedded length, and mechanical properties of the cement matrix on the pull-out mechanisms of the CNT from the cement matrix, the debonding process at the interface between the CNT and the matrix, and the nano-crack initiation and propagation in the cement matrix surrounding the CNT. This will be achieved through an idealized finite element analysis of a unit cell which contains an embedded single straight CNT in a cement matrix where the pull-out process of the CNT from the cement matrix is simulated using a phenomenological continuum-based model. In this paper, the CNT is modeled as an isotropic linear elastic shell, the cement matrix is modeled using a coupled elasto-plastic-damage model formulated by Abu Al-Rub and Kim [3], and the interface is modeled using a cohesive surface model. To the authors' best knowledge, this computational framework has not been attempted before for CNT/cement composites. However, in this study, interfacial friction after debonding is neglected and will be the focus of a future study.

2. Finite Element Model

Fig. 1 shows a unit cell model for the CNT/cement matrix composite which contains a single straight CNT embedded in the cement matrix. The outer diameter, thickness, and embedded length of the CNT are assumed to be 20, 0.34, and 1000 nm, respectively. The diameter of the cement matrix surrounding the CNT is assumed 292 nm.

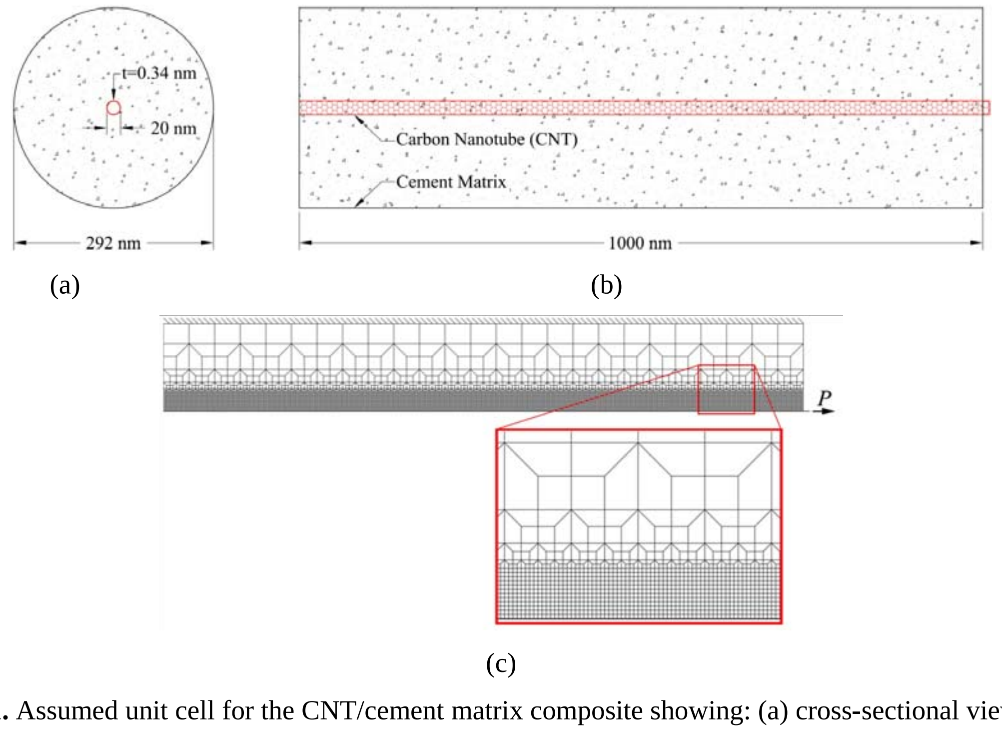

Fig. 1. Assumed unit cell for the CNT/cement matrix composite showing: (a) cross-sectional view, (b) side view, and (c) finite element mesh and imposed boundary conditions.

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Since both the CNT and cement matrix are axisymmetric with respect to the longitudinal axis, an axisymmetric finite element model is generated as shown in Fig. 1(c) where the CNT is subjected to a pulling force. The commercial finite element software Abaqus is used for the analysis. A 4-node bilinear axisymmetric quadrilateral element with reduced integration (CAX4R) is used for the cement matrix and a 2-node linear axisymmetric shell element (SAX1) is used for the CNT. The minimum element size of cement matrix is 2.5 nm × 2.5 nm, and mesh density is coarsened towards outer surface boundary in order to reduce the analysis time.

The coupled elastic-plastic-damage model formulated by Abu Al-Rub and Kim [3] based on laws of thermodynamics and continuum damage mechanics is used here for modeling the nonlinear behavior of the cement matrix. Therefore, one can consult [3] for the detailes of the model used to simulate the damage behavior of the cement matrix. On the other hand, the interface between the CNT and the cement matrix is modeled using the well-known cohesive surface models. Since the interface between the CNT and cement matrix has almost a zero thickness, then a surface-based cohesive behavior (versus a cohesive zone of finite thickness [4] in which the zone thickness is a constitutive parameter), which is primarily intended for simulations in which the thickness of the interface is negligibly small, is adopted here.

There are many cohesive surface models that exist in the literature of which several are available in Abaqus [4]. For simplicity, as shown in Fig. 2, the cohesive surface model is described in this study by a linear elastic traction-separation law prior to damage (i.e., up to the cohesive strength t^0) and a damage evolution with linear softening as the displacement jump across the interface (i.e., the separation δ) increases. The cohesive bond is characterized by a progressive degradation of the cohesive stiffness K by the damage variable D where complete separation occurs once $\delta \geq \delta^f$. The cohesive bond energy, G, which is referred to here as the interfacial fracture energy and dissipates upon complete debonding, is the area under the traction-separation curve.

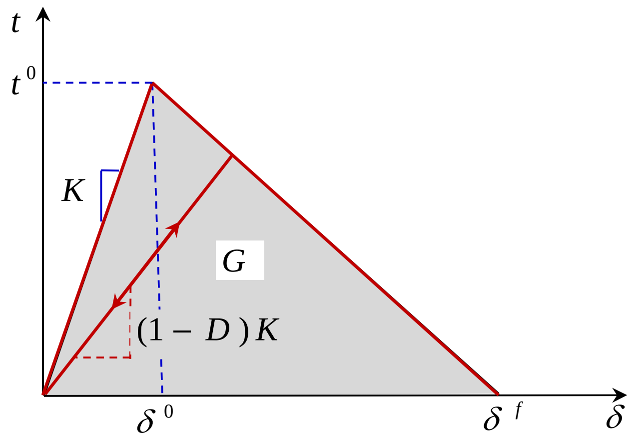

Fig. 2. Typical linear cohesive surface model.

The key interfacial properties in the adapted cohesive surface model are the initial cohesive stiffness, $K = t^0/\delta^0$, the cohesive strength, t^0, and the interfacial fracture energy, G. Note that the cohesive surface properties introduce a length scale $\delta_m^f - \delta_m^0$ (i.e., the difference between the equivalent separation at complete debonding to that at damage initiation); therefore, what matters in the calculations is the ratio of geometric lengths to this length scale.

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The elastic properties of the CNT are taken to be $E_{CNT} = 1000\,\text{GPa}$ and $\nu_{CNT} = 0.3$. The material parameters associated with the elastic-plastic-damage model for the cement matrix that are used in the analysis are taken from Kim and Abu Al-Rub [5].

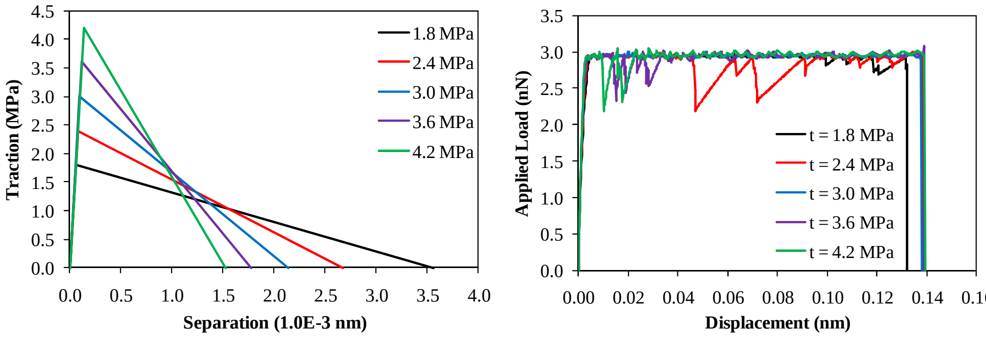
3. Parametric Study

3.1 The effect of the interfacial shear strength

The effect of the interfacial shear strength, t_s^0, on the CNT's pull-out force (strength) and debonding displacement (ductility) is investigated. Generally, larger pull-out force and debonding displacement indicate, respectively, stronger/stiffer and more ductile nanocomposite cement. Therefore, it imperative to investigate the key parameters that increase both pull-out force and debonding displacement simultaneously. Now, in order to investigate the effect of only t_s^0, other interfacial properties, such as the cohesive stiffness K and the fracture energy G, are kept constant. Currently, to the authors' best knowledge, experimental studies about the interfacial strength of the CNT/cement composites are not available yet. Thus, the range of t_s^0 extracted from the pull-out experimental test by Naaman et al. [6] is used here. Naaman et al. [6] investigated the pull-out strength and the interfacial bond shear stress through the pull-out test of a single macro steel fiber embedded in a cementitious matrix, and the test showed that the t_s^0 varies from 1.47 MPa (for low strength cement) to 9.73 MPa (for high strength cement). These values are much lower than the values of the interfacial strength of multi-wall carbon nanotubes in a polethylenebutene matrix (47 MPa) obtained using an atomic force microscope tip-based pull-out experiment [2] and 170 MPa for carbon nanofibers in an epoxy matrix obtained using an *in-situ* (i.e., direct visualization) single fiber pull-out test [1].

Fig. 3 shows the assumed variation of t_s^0 and its effect of the single CNT pull-out behavior while keeping G and K constant. t_s^0 is assumed to vary between 1.8 MPa to 4.2 MPa with an increment of 0.6 MPa while G is assumed 32×10^{-16} N/nm. As shown from Fig. 3(b), the pull-out force and debonding displacement are merely affected by the variation of t_s^0. In the meanwhile, the increase of G increases the CNT pull-out force and debonding displacement simultaneously.

It is noteworthy that t_s^0 does not have a significant effect on the damage evolution in the cement matrix when G is fixed; although, sudden drops in the pull-out force can be seen due to nano-cracks initiation and evolution within the cement matrix as shown in Fig. 3(b). It should also be noted that there are two reasons causing the drop of the applied load during the pull-out process; one is due to damage evolution in the cement matrix and the other is due to the accumulated interfacial energy release. In the case of $t_s^0 = 2.4\,\text{MPa}$, the pull-out force shows several sudden drops due to damage evolution in the cement matrix such that one can notice that the interfacial shear stiffness during reloading, as compared to the initial elastic shear stiffness of the interface, reduces as the pull-out displacement increases. On the other hand, the sudden drop in the pull-out force when t_s^0 is 3.6 MPa and 4.2 MPa is due to the abrupt interfacial energy release.



(a) (b)

Fig. 3. (a) The effect of the interfacial shear strength t^0 on the (b) pull-out force and debonding displacement while fixing the interfacial stiffness and facture energy.

Fig. 4 shows the damage initiation and evolution in the cement matrix during the pull-out process for $t_s^0 = 3.6\,\text{MPa}$ and $G = 16\times10^{-16}\,\text{N/nm}$. However, the level of damage in the cement matrix in close proximity of the CNT is not that significant since the interfacial shear strength (3.6 MPa) is slightly higher than the cement's tensile strength (3 MPa). Therefore, one expects that as the interfacial strength increases, more damage occurs within the cement matrix as the stresses around the CNT would cause the cement matrix to crack before the interface. As seen from Fig. 4, the first drop in the pull-out force is not caused by the matrix damage, but caused by the strain energy release, whereas the second drop of the applied load is due to nano-crack initiation in the cement matrix when the CNT is pulled-out 0.027nm displacement. Fig. 4 shows several nano-cracks that are initiated and propagated within the cement matrix during further pull-out of the CNT. The nano-cracks are aligned perpendicular to the CNT's length. The final debonding is shown in Fig. 4 with several damage regions along the length of the CNT. The spacing between the evolved nano-cracks is not uniform, but tends to localize at some regions.

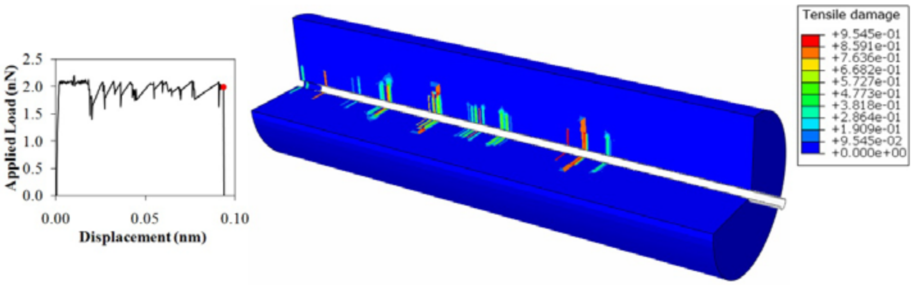
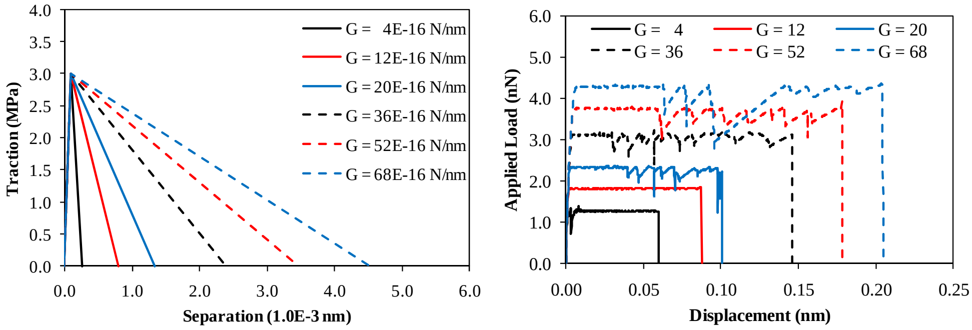


Fig. 4. The damage evolution in the cement matrix at the end of pull-out process for $t^0 = 3.6\,\text{MPa}$ and $G = 16\times10^{-16}\,\text{N/nm}$.

3.2 The effect of the interfacial fracture energy

It would be interesting to investigate the effect of varying the interfacial fracture energy G on the CNT's pull-out force and debonding displacement while fixing t^0 and K (or equivalently δ^0). Fig. 5(a) shows the corresponding assumed traction-separation curves while setting $t^0 = 3\text{MPa}$. Note that the slope of the linear softening part of the traction-separation curves is changed so that the fracture energy varies from 4×10^{-16} N/nm to 68×10^{-16} N/nm.

The results of the fracture energy sensitivity analysis are shown in Fig. 5(b). One can clearly see that both the CNT's pull-out force and debonding displacement are proportional to the fracture energy. The pull-out strength and debonding displacement of the CNT increase almost linearly as the fracture energy increases such that the same fracture energy gives almost the same pull-out force and debonding displacement regardless of the interfacial shear strength or cohesive stiffness. It means that the composite strength between the CNT and cement matrix is governed by the fracture energy of the interface rather than by the interfacial shear strength or the cohesive stiffness. Also, one notices from the fluctuation in the pull-out force that more damage is induced in the cement matrix as G increases. This implies that more stresses are transferred to the cement matrix as the interfacial bond energy between the CNT and the cement matrix is increased. Therefore, one may argue that enhancing G may increase the overall strength and ductility of the nanocomposite cement material.



(a) (b)

Fig. 5. (a) The effect of the interfacial fracture energy G (x10^{-16} N/nm) on the (b) pull-out force and debonding displacement while fixing interfacial stiffness and strength.

4. Conclusions

This paper focuses on investigating the key parameters that control the pull-out behavior of a single straight CNT from a cement matrix. The effects of interfacial properties (interfacial shear strength, interfacial bond energy) have been investigated. In this study, while the variations of the interfacial shear strength and cohesive stiffness have merely affected the CNT's pull-out force (strength) and the debonding displacement (ductility), the pull-out behavior is strongly governed by the interfacial fracture energy (or cohesive energy which is the area under the traction-separation curve). Therefore, the common argument in the literature that in order to enhance the bonding between the CNT and a matrix material the interfacial shear strength is the key controlling parameter might not be that accurate as this depends on whether the cohesive energy is equally increased or not. In fact, the interfacial shear strength is an important interfacial property as long as the cohesive energy is enhanced. Thus, for the sake of assessing the potential of different CNT's surface modifications in order to enhance the bond between CNTs and the host cement matrix, it is imperative to measure both the interfacial strength and interfacial energy in order to make such an assessment a meaningful one.

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References

[1] Manoharan MP, Sharma A, Desai AV, M.A. H, Bakis CE, Wang KW. The interfacial strength of carbon nanofiber epoxy composite using single fiber pullout experiments. Nanotechnology. 2009;20:295701.

[2] Barber AH, Cohen SR, Wagner HD. Measurement of carbon nanotube-polymer interfacial strength. Appl Phys Lett. 2003;82:4140–2.

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[3] Abu Al-Rub RK, Kim S-M. Computational applications of a coupled plasticity-damage constitutive model for simulating plain concrete fracture. Engineering Fracture Mechanics. 2010;77:1577-603.
[4] 6.9 A. Abaqus User's Manual. Providence, RI: Dassault Systèmes/SIMULIA; 2009.
[5] Kim S-M, Abu Al-Rub RK. Meso-scale computational modeling of the plastic-damage response of cementitious composites. Cement and Concrete Research. 2011;41(3):339-58.
[6] Naaman AE, Namur GG, Alwan JM, Najm HS. Fiber pullout and bond slip. II: Experimental validation. ASCE Journal of Structural Engineering. 1991;117:2791-800.

Excerpt from ISBN 978-3-00-053387-7