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A numerical study on carbon nanotube pullout to understand its bridging effect in carbon nanotube reinforced composites

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Carbon nanotube (CNT) reinforced polymeric composites provide a promising future in structural engineering. To understand the bridging effect of CNT in the events of the fracture of CNT reinforced composites, the finite element method was applied to simulate a single CNT pullout from a polymeric matrix using cohesive zone modelling. The numerical results indicate that the debonding force during the CNT pullout increases almost linearly with the interfacial crack initiation shear stress. Specific pullout energy increases with the CNT embedded length, while it is independent of the CNT radius. In addition, a saturated debonding force exists corresponding to a critical CNT embedded length. A parametric study shows that a higher saturated debonding force can be achieved if the CNT has a larger radius or if the CNT/matrix has a stronger interfacial bonding. The critical CNT embedded length decreases with the increase of the interfacial crack initiation shear stress.

1. Introduction

Nanocomposite is a multiphase solid material where one of the reinforcing materials is less than 100 nm [1]. Polymeric nanocomposite materials, which combine polymers with nanoadditives, have attracted vast interest as a new material with many uses [2–4]. CNTs are the finest and strongest fibres with nanoscale diameter and length ranging from micro to millimetres [5]. They were discovered by Iijima in 1991 [6]. They are the ideal reinforcement for high performance composites due to their small size, low density, high stiffness and high strength; and therefore, considered as the new generation of reinforcing phase in fabricating nano-composite materials. Measurements used *in situ* transmission electron microscopy and atomic force microscopy show that the Young's modulus of CNTs is in the order of 1 TPa [7,8]. The tensile strength is up to 150 GPa [9]. CNTs are currently used in both conventional and novel areas, such as lightweight structural composites, field emission devices, and electronics. In the past few years, research has been carried out to better understand the mechanical performance of CNT reinforced composites. It showed that a small quantity of nanotubes added to a polymer matrix can increase the stiffness and strength of the composite [3,4]. For example, dispersing 1% wt of CNTs to a matrix material results in up to 42% increase in the stiffness of the composite [3]. However, it is difficult to control the alignment and orientation of the CNTs in directly dispersing of CNTs to the resin; therefore, it has the difficulty to control the quality of the produced CNT-based composites.

Fracture toughness is one of the most important properties in many applications. Recently, some experimental studies have shown that using CNTs as the reinforcement can improve the fracture toughness [10–15]. The toughening mechanisms depend critically on the CNT/matrix interfacial behaviour which can be investigated through a CNT pullout test [16–19]. However, due to their extremely small size, only a few experimental studies have been carried out. Echeberria et al. [13] reported an increase in fracture toughness of multi-walled carbon nanotubes and single-walled carbon nanotubes reinforced alumina composites. They indicated that the pullout of CNTs and bridging are the reasons of the improved fracture toughness. Barber et al. [17] investigated the interfacial fracture energy using a single multi-walled CNT pullout test from a polymer matrix at a short embedded length. Their results suggested that a relatively strong interface with a high fracture energy. Lachman and Wagner [19] also found that the nanocomposite toughness increases with enhanced interfacial adhesion. They explained this result by using a pullout energy model and found that the pullout energy increases with the interfacial shear strength.

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Besides the experimental work, many theoretical studies have been carried out to understand the mechanical performance of CNT reinforced composites [16,20–23]. Various approaches have been proposed by using molecular dynamic (MD) simulation [16,20,22,23]. For example, using molecular mechanics simulation, Liao and Li [16] investigated the interfacial characteristics of CNT reinforced polystyrene composite from pullout, including thermal residual radial stress, pullout energy and interfacial shear stress. Their result showed that the estimated interfacial shear stress (τ_s = 160 MPa) is significantly higher than most carbon fibre reinforced polymer composite. Zheng et al. [20] used both molecular mechanics and MD simulations to estimate the interfacial shear strength, which is about 33 MPa. However the length of the CNT in the MD models was limited to the range of 4–10 nm due to the intensive computational requirements in the MD simulations [16,23–25].

The typical length of CNTs is in the order of a few microns, while the diameters range from less than 1 nm to about 30 nm that corresponds to an aspect ratio around 1000 [26]. The fracture toughness has the potential to be improved by increasing the CNT embedded length (interface length L_{CNT}) because of the increased interfacial area and therefore, increased energy dissipation. However, Chen et al. [27] carried out a theoretical study which showed that longer reinforcing CNTs do not definitely provide better fracture toughness on composites. For a strong adhesion between CNT and matrix, CNTs are fragmented with an increase in CNT length, which results in a sudden drop of the fracture toughness. In a weak adhesion between CNT and matrix interface, although the CNTs are pulled out, the improvement of fracture toughness quickly becomes saturated with an increase in CNT length.

To understand the bridging effect of CNT in the events of the fracture of CNT-reinforced composites, this paper investigates the single CNT pullout test by using cohesive zone modelling. The effect of interfacial bonding between CNT and epoxy matrix as well as CNT geometry effect on the debonding force are investigated, particularly on the effect of CNT embedded length. The bridging resistance of CNT is quantified by the specific pullout energy, pullout energy per unit interfacial area, in this research.

2. Finite element model for CNT pullout

Due to the limitations of computing time and resources of using MD method to study the pullout of CNTs, the finite element method is used to simulate the single CNT pullout at microscale in current study. In some other studies, CNTs have been described as a continuum solid beam or shell subjected to tension, bending, or torsional forces by applying continuum mechanics [25,26,28,29]. In this study, the continuum mechanics was applied to treat CNTs as membranes. Therefore, the nanoscale dimension of the wall thickness of the CNTs was excluded in the simulations. The nano- and the microscales problem becomes a single microscale problem.

In the single CNT pullout, a two-dimensional axisymmetric model at microscale was developed using a single cylindrical CNT embedded in a semi-infinite matrix. A pullout displacement was applied on the top of the CNT in the axial direction, as shown in Fig. 1(a). In this study, a 24 nm diameter carbon nanotube is embedded in an epoxy matrix with the embedded length L_{CNT} = 2.6 μm, which is consistent with the experiment by Cooper et al. [30]. The CNT and epoxy matrix were modelled as isotropic materials. The Young's modulus of CNT was taken as E_{CNT} = 1.1 TPa with the wall thickness = 0.34 nm, and epoxy matrix with E_m = 3.4 GPa was used in this study. The elastic Poisson's ratios of CNT ν_{CNT} and matrix ν_m, were kept respectively constant as 0.34

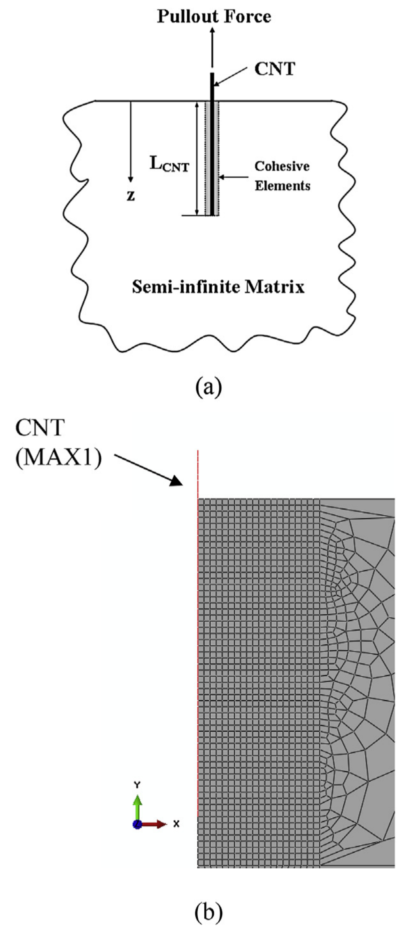

Fig. 1. (a) A schematic diagram of a single CNT pullout model; (b) Axisymmetric finite element model for a single CNT pullout: fine mesh around the interface.

and 0.36 in all simulations. Membrane elements (MAX1) were used in commercial finite element package Abaqus to represent the cylindrical CNT as shown in Fig. 1(b). Membrane elements can be used to represent a thin surface in space which offers strength in the plane of the element without bending stiffness [31]. In addition, the axisymmetric cohesive elements (COHAX4) were used to define the cohesive zone between the interface of the CNT and the matrix.

Cohesive zone modelling is a commonly used technique to investigate the failure governed by crack or debonding propagation [32–34]. It uses the traction stress as a function of the separation at any point along a potential fracture path to describe the physical debonding/cracking process at that point. The area under the traction–separation curve is the fracture energy release rate, which is consistent with the concept in fracture mechanics to represent the energy required to create a unit fracture surface area. However, little attention has been paid to use cohesive zone modelling to simulate fibre pullout. Some researchers have derived the cohesive law for the CNT/polymer interface from the analysis of the weak van der Waals bonds [35–37]. The limitation of these analytical studies is that the cohesive laws derived are for an infinite length of CNT embedded in a polymer matrix. In addition, these proposed cohesive laws are too complicated to be applied in a finite element simulation. In this study, a cohesive zone model was adopted from Tvergaard [38] and Chaboche et al. [39]. As the previous study [40], a simplified cohesive zone model was used as