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A numerical study on carbon nanotube–hybridized carbon fibre pullout

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ABSTRACT

Carbon nanotube (CNT)–hybridized carbon fibre (CF) composite is a new generation composite, where CNTs grow radially on carbon fibres to form a hybrid reinforcing phase. To evaluate the bridging effect of this new reinforcing phase, a numerical method is proposed to theoretically investigate the pullout of a hybrid fibre. There are two finite element models developed in this method, which are applied to simulate a single CNT pullout from the matrix at microscale and the pullout of the hybrid fibre at macroscale. The bridging effect of the CNTs during the hybrid fibre pullout is simulated by spring elements in the macroscale finite element model, where the properties of spring elements are obtained from the microscale finite element simulation. The numerical results indicate that the apparent interfacial shear strength of the hybrid fibre and the specific pullout energy can be significantly increased due to the additional bonding of the CNT–matrix interface. A parametric study indicates that the bridging effect of the hybrid fibre can be further enhanced by improving the interfacial bonding between CNT and matrix and increasing the size or length of CNTs. This study provides a new numerical method to simulate the multiscale CNT/CF hybrid fibre pullout.

1. Introduction

Carbon nanotubes (CNTs) are the finest and strongest fibres with a nanoscale diameter and length ranging from micro- to millimetres [1]. CNTs are widely used in many areas, such as electronics, nano-electro-mechanical devices and medical applications. In the past few years, studies have 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 [2,3]. For example, dispersing 1 wt% of CNTs to a matrix material results in up to 42% increase in the stiffness of the composite [2]. However, directly dispersing CNTs to the resin has difficulty in controlling the alignment and orientation of the CNTs and, therefore, there will be difficulties in controlling the quality of the produced CNT-based composites.

A recent development of CNT composites is through chemical vapour deposition (CVD) to grow CNTs radially on micro-fibres, such as carbon fibres, and to use these hybrid fibres to develop superior 3D composites, carbon nanotube (CNT)/carbon fibre (CF) hybrid composites [4]. CNT/CF hybrid composites combine the advantages of both the carbon fibres and the carbon nanotubes. Because traditional fibres only provide in-plane reinforcement, delamination can easily occur since there is no reinforcement in the direction of the z coordinate (through-thickness direction) to resist crack initiation and propagation. Since the CNTs align in multi-directions in the matrix, they can provide reinforcement to the matrix in different directions as a 3D reinforcement. Due to the extremely high tensile strength, stiffness and the increased interfacial area, it is expected that the fracture toughness of the new composites with the hybrid 3D reinforcement will be increased substantially.

The performance of a composite critically depends on the interfacial properties between the reinforcing phase and the matrix phase. Interfacial shear strength is a key parameter to determine the efficiency of load transfer from the polymer matrix to the fibres. Recent results have shown the improvement of the interfacial strength between the fibres and matrix by growing CNTs on the surfaces of carbon fibres [4–8]. A single fibre pullout test is one of the widely used techniques to quantify the interfacial strength. A few studies have been carried out to understand the mechanical performance of CNTs reinforced composites using the single fibre pullout test [9–11].

In comparison to experimental research, theoretical and numerical analysis can provide additional insight into the reinforcing effect of CNTs-based nanocomposites, which can assist the further development and design optimisation of composites. Several numerical studies have been carried out on the CNT pullout [12–15], but no numerical study on CNT/CF hybrid fibre pullout has been reported. It is due to the complexity of pullout process of the hybrid fibre and the two different scales of the CNTs and

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the fibre–matrix. Kulkarni et al. [16] and Nie et al. [17] developed two similar multiscale models to evaluate the effect of interfacial strength on the elastic modulus of hybrid fibre reinforced polymer composites. They firstly modelled a nanocomposite formed by a single CNT–matrix and numerically predicted the overall mechanical properties of the nanocomposite. The second step is to consider the nanocomposite as an equivalent matrix and use it to form a single carbon fibre nanoreinforced laminated composite. No CNT/CF hybrid fibre pullout was studied in these two papers.

The purpose of this paper is to develop a numerical method to simulate the pullout of a single CNT/CF hybrid fibre. The interfacial bonding between the hybrid fibre and the matrix, and the bridging effects of the hybrid fibre on the composite are able to be theoretically examined by using this method. The bonding and debonding behaviours between the carbon fibre–matrix interface and between the CNT–matrix interface are described by cohesive laws. In addition, the effect of relevant parameters of CNTs on the hybrid fibre pullout behaviour is discussed.

2. Numerical method for hybrid fibre pullout

CNTs can be radially grown on the surface of carbon fibres and then embedded in an epoxy matrix to produce CNT/CF hybrid fibre reinforced composite, as shown in Fig. 1(a) [11]. During the hybrid fibre pullout, there are two types of interfaces, carbon fibre–matrix interface and CNT–matrix interface. As the pullout force is applied to the carbon fibre, both shear and tensile load can be transferred to the CNTs. The stresses in the CNTs will be transferred to the matrix through CNT–matrix interface. As the pullout force increases, cracks initiate and propagate along both interfaces of carbon fibre–matrix and CNT–matrix, which leads to the debonding of the carbon fibre–matrix interface and CNT–matrix interface.

To numerically simulate the complicated hybrid fibre pullout, a few assumptions are made to simplify the problem:

(1) It is assumed that the CNTs are uniformly grown on the carbon fibre and they are ideally aligned in the radial direction. As shown in Fig. 1(a), CNTs are densely distributed on the fibre, and therefore, the assumption of the uniform CNTs distribution is acceptable. Due to the large amount of CNTs, the effects of the curvature and the direction misalignment of individual CNTs are almost impossible to simulate and therefore, these effects are neglected in this theoretical study.
(2) All the CNTs are assumed to have identical geometry (including the radius and the length) and mechanical property. The bonding and debonding behaviour of the interfaces between individual CNTs and the matrix is also assumed to be the same. Based on this assumption, the bridging effects of all the CNTs are identical and only a single CNT pullout study is needed.
(3) Possible matrix damage during the hybrid fibre pullout is neglected in this numerical study.

Based on these assumptions, an idealized hybrid fibre pullout problem is illustrated in Fig. 1(b).

During the single CNT/CF hybrid fibre pullout, there are two physical phenomena, which occur at two different scales: CNT pullout at microscale and carbon fibre pullout at macroscale. To overcome the difficulties in the simulation of the multiscale problem, a numerical method is proposed to deal with the two pullout processes explicitly but in two separate finite element models. A finite element model at microscale is applied to simulate a single CNT pullout from the matrix and another finite element model at macroscopic scale is applied to simulate the pullout of the hybrid fibre. The bridging effect of the CNTs during the hybrid fibre pullout is simulated by using equivalent spring elements in the macroscale hybrid fibre pullout model, where the spring elements' property is obtained from the microscale CNT pullout simulation.

2.1. Finite element model for CNT pullout at microscale

Some numerical methods have been developed to study the CNT–matrix interface by using the molecular dynamic (MD) method and the finite element method. Examples on the study of using the MD method can be found in [12,15,18,19], where the bonded and nonbonded potentials are represented in terms of the force constants and the change in distance among the atomic bonds. However the length of the CNT in the MD models is limited to the range of 4–10 nm because of the intensive computational requirements in the MD simulation [13,15,16,20]. Due to this limitation, applying MD method to study the pullout of CNTs with the length in several micrometres is unachievable. On the other hand, CNTs have been described as a continuum solid beam or shell subjected to tension, bending, or torsional forces by applying continuum mechanics [14,20,21]. In this way, the nanoscale dimension in the thickness direction of the CNTs is not explicitly involved in the models. The nano- and the microscales problem becomes a single microscale problem. In the current study, the continuum mechanics is applied to treat CNTs as membranes.

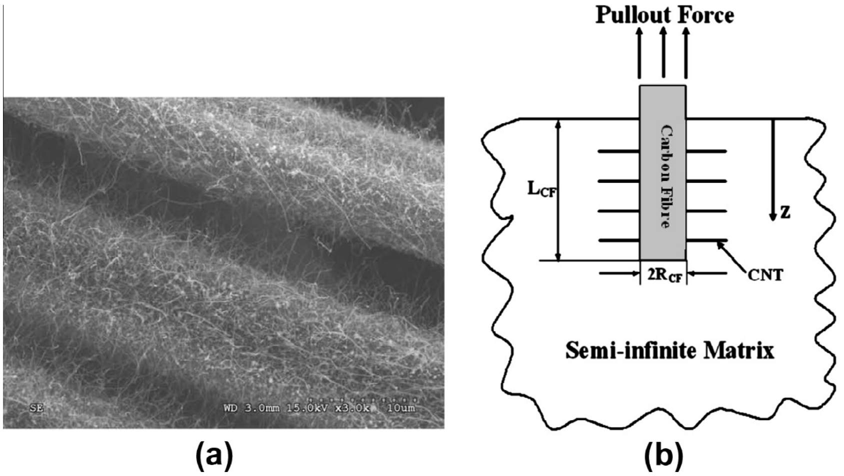

Fig. 1. (a) SEM image of hybrid fibres with CNTs [11]; and (b) a schematic diagram of the idealized CNT/CF hybrid fibre pullout problem.